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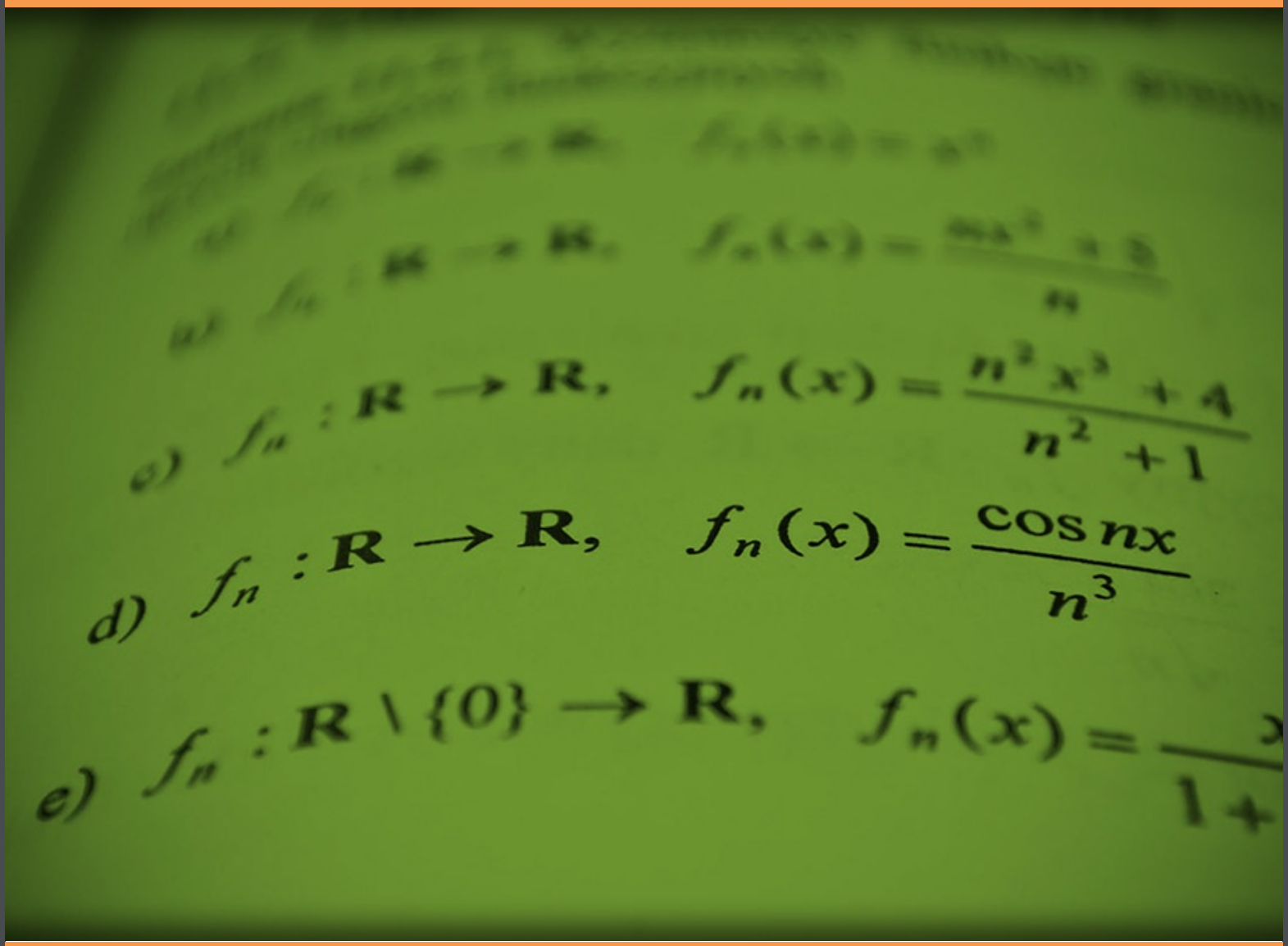
Introduction to Lagrangian & Hamiltonian Mechanics

Jacob Linder; Iver H. Brevik


$f_n : \mathbf{R} \to \mathbf{R}, \quad f_n(x) = \frac{n^2 x^3 + 4}{n^2 + 1}$
$f_n : \mathbf{R} \to \mathbf{R}, \quad f_n(x) = \frac{\cos nx}{n^3}$
$f_n : \mathbf{R} \setminus \{0\} \to \mathbf{R},$

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Introduction to Lagrangian & Hamiltonian Mechanics

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Introduction to Lagrangian & Hamiltonian Mechanics
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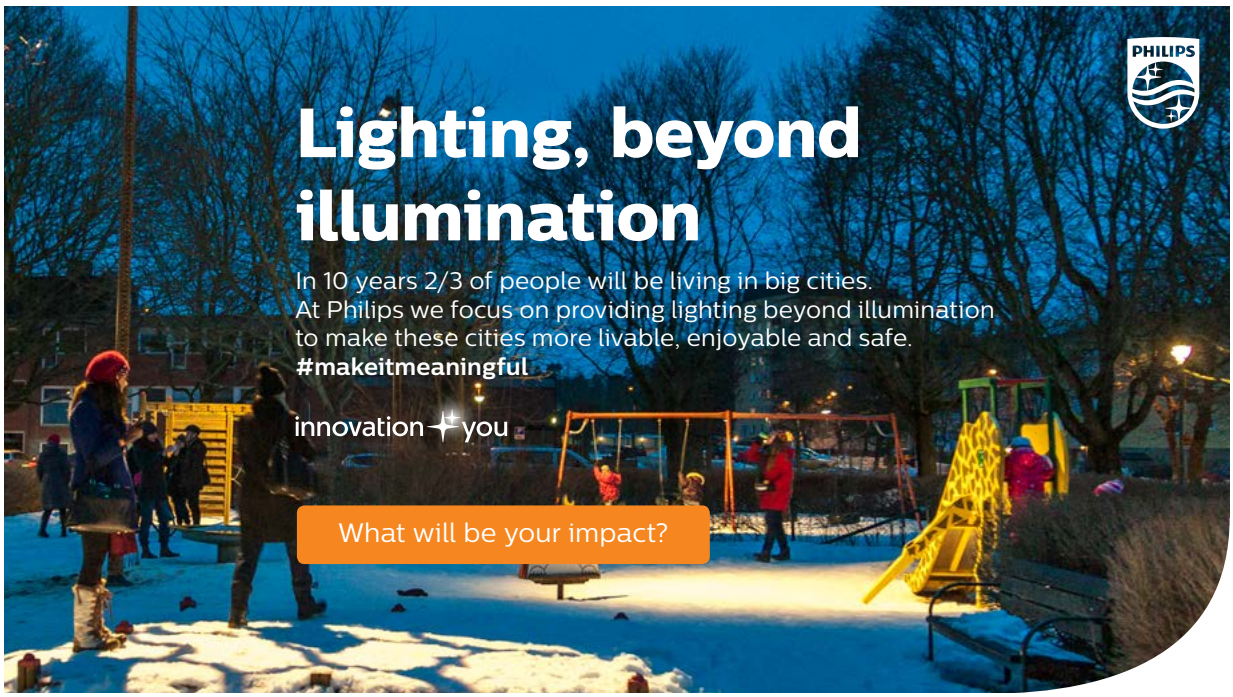
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Preface

In both classical and quantum mechanics, the Lagrangian and Hamiltonian formalisms play a central role. They are powerful tools that can be used to analyze the behavior of a vast class of systems, ranging from the motion of a single particle in a static potential field to complex many-body systems featuring a strong time-dependence.

The aim of this book is to provide an introduction to the Lagrangian and Hamiltonian formalisms in classical systems. We will cover both non-relativistic and relativistic systems. This presentation is prepared with an undergraduate audience in mind, typically a student at the end of the first or beginning of the second year. In addition to explaining the underlying theory in a detailed manner, we shall also provide a number of examples that will illustrate the formalisms "in action".

These lecture notes are primarily based on the teaching of I.B. and follows to some extent also the structure of the excellent textbook by Goldstein *et al.* "Classical Mechanics". We have also included some examples not found in Goldstein inspired by instructive examples found in other lecture notes, all of which have been properly cited where they appear. Special thanks goes also to Jon Andreas Støvneng and Simen Ellingsen for their contribution to the lecture notes in this course over the years.

The lectures given in this course given by J.L. have been recorded on video and uploaded on YouTube. Thus, at the beginning of each chapter we provide a link to the YouTube-videos covering that particular chapter. Here is the complete playlist of YouTube-videos covering all topics in this book.

It is our goal that students who study this material afterwards will find themselves well prepared to dig deeper into the remarkable world of theoretical physics at a more advanced level. We have carefully chosen the topics of this book to make students proficient in using and understanding important concepts such as symmetries and conservation laws, the special theory of relativity, and the Lagrange/Hamilton equations.

We welcome feedback on the book (including any typos that you may find, although we have endeavored to eliminate as many of them as possible), and hope that you will have an exciting time reading it!

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About the authors

J.L. holds since 2013 a position as Professor of Physics at the Norwegian University of Science and Technology. His research is focused on theoretical quantum condensed matter physics and he has received several prizes for his Ph.D work on the interplay between superconductivity and magnetism. He has also received the American Physical Society ”Outstanding Referee” award, selected among over 60.000 active referees. In teaching courses such as Classical Mechanics and Particle Physics for both undergraduate and graduate students, he has invariably received high scores from the students for his pedagogical qualities and lectures. His webpage is found here.

I.B. has for about 20 years been a Professor of Mechanics at the Norwegian University of Science and Technology. He has worked within electrodynamics, fluid mechanics, and cosmology, and has alone or with co-authors published about 250 research papers in international journals. He was a member of the Editorial Board of Physical Review E, in the period 2009-2014, and was awarded the American Physical Society's ”Outstanding Referee”, at their first round in 2008. The present book actually grew out from a course of lectures given by him on Classical Mechanics at the university during a period of about 15 years. His webpage is found here.

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I. FUNDAMENTAL PRINCIPLES

Youtube-videos. 01-04 in this playlist.

Learning goals. After reading this chapter, the student should:

- Know how to construct the Lagrange function for a system
- Be able to write down and solve Lagrange's equations
- Know how to incorporate friction in the Lagrangian formalism

A. Notation and brief repetition

To begin with, let us establish some notation for the various physical quantities that will appear throughout this book. The velocity vector is denoted $\boldsymbol{v} = d\boldsymbol{r}/dt$, linear momentum $\boldsymbol{p} = m\boldsymbol{v}$, force $\boldsymbol{F}$, angular momentum $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$, angular torque $\boldsymbol{\tau} = \boldsymbol{r} \times \boldsymbol{F}$. From basic mechanics, we know that Newton's 2nd law reads:

$$\boldsymbol{F} = \frac{d\boldsymbol{p}}{dt} \tag{1.1}$$

and is valid in inertial systems. For now, we may think of an inertial system as a non-accelerated system, meaning that objects will move in straight lines at constant velocity unless acted upon by some force. In the special case of a constant mass m, the 2nd law may be written as $\boldsymbol{F} = m\boldsymbol{a}$ where $\boldsymbol{a}$ is the acceleration.

There is also an "equivalent"' of Newton's 2nd law which is useful for rotational motion. Consider the torque $\boldsymbol{\tau}$:

$$\begin{aligned}\boldsymbol{\tau} = \boldsymbol{r} \times \frac{d\boldsymbol{p}}{dt} = \frac{d}{dt}(\boldsymbol{r} \times \boldsymbol{p}) - \frac{d\boldsymbol{r}}{dt} \times \boldsymbol{p} = \frac{d\boldsymbol{L}}{dt} - \boldsymbol{v} \times m\boldsymbol{v} \\ = \frac{d\boldsymbol{L}}{dt}.\end{aligned} \tag{1.2}$$

It follows from equation (1.1) that if $\boldsymbol{F} = 0$, then $\boldsymbol{p}$ is conserved (time-independent). Similarly, it follows from equation (1.2) that if $\boldsymbol{\tau} = 0$, then $\boldsymbol{L}$ is conserved. We will have much more to say about such conservation laws later on in this book. As a final preliminary, we also briefly remind the reader of the meaning of a conservative system. The work done by a force $\boldsymbol{F}$ on particle moving from point 1 to 2 is defined as:

$$W_{12} = \int_1^2 \boldsymbol{F} \cdot d\boldsymbol{s} \tag{1.3}$$

where $d\boldsymbol{s}$ is an infinitesimal displacement along the trajectory of the particle. If we for simplicitly assume that m is constant, we get

$$\int \boldsymbol{F} \cdot d\boldsymbol{s} = m \int \frac{d\boldsymbol{v}}{dt} \cdot \boldsymbol{v} dt = m\frac{1}{2} \int \frac{d}{dt} v^2 dt. \tag{1.4}$$

The result is then $W_{12} = \frac{1}{2}m(v_2^2 - v_1^2) = T_2 - T_1$. In effect, the work performed on the particle equals the change in the kinetic energy of the particle. The system is said to be *conservative* if the work performed between points 1 and 2 is independent of which path one takes between them. Put mathematically, we would write that:

$$\oint \boldsymbol{F} \cdot d\boldsymbol{s} = 0, \tag{1.5}$$

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which implies that the force can be written as $\boldsymbol{F} = -\nabla V(\boldsymbol{r})$. Here, V is the potential energy which can depend on the position $\boldsymbol{r}$. Note that we can always choose the reference level of zero energy for the potential energy as we please, because adding a constant V_0 to V does not change the physical force: $\boldsymbol{F} = -\nabla[V(\boldsymbol{r}) + V_0] = -\nabla V(\boldsymbol{r})$ since $\nabla V_0 = 0$. We mention in passing that a system including friction cannot possibly be conservative, since the net work done upon completing a closed trajectory starting at point 1 and ending up at the same point 1 must be positive, in contrast to equation (1.5).

At this stage, we have two expressions for the work performed on particle moving from point 1 to 2:

$$W_{12} = T_2 - T_1 = V_1 - V_2 \rightarrow T_1 + V_1 = T_2 + V_2. \tag{1.6}$$

In other words:

$$\boxed{\text{The total energy } T + V \text{ is constant for a conservative system}}.$$

B. Many-particle systems

In a system with many particles, Newton's 2nd law must take into account both external forces and all forces from interactions in the system. For particle i, we get:

$$\boldsymbol{F}_i^{\text{ext}} + \sum_j \boldsymbol{F}_{ji} = \dot{\boldsymbol{p}}_i. \tag{1.7}$$

Here, $\boldsymbol{F}_i^{\text{ext}}$ is the external force acting on particle i while $\boldsymbol{F}_{ji}$ is the internal force acting on particle i due to particle j. Assuming that $\boldsymbol{F}_{ji}$ satisfies Newton's 3rd law, it has to be equal in magnitude but opposite in direction of $\boldsymbol{F}_{ij}$. Thus, we get $\boldsymbol{F}_{ij} = -\boldsymbol{F}_{ji}$. Using this and performing a summation over all particles i, equation (1.7) becomes:

$$\frac{d^2}{dt^2}\sum_i m_i \boldsymbol{r}_i = \underbrace{\sum_i \boldsymbol{F}_i^{\text{ext}}}_{\text{Total external force } \boldsymbol{F}^{\text{ext}}} + \underbrace{\sum_{\substack{i,j \\ i \neq j}} \boldsymbol{F}_{ji}}_{=0}. \tag{1.8}$$

We define the center of mass (CM) position $\boldsymbol{R}$:

$$\boldsymbol{R} = \frac{\sum m_i \boldsymbol{r}_i}{\sum m_i} = \frac{\sum m_i \boldsymbol{r}_i}{M}. \tag{1.9}$$

Using $\boldsymbol{R}$, Newtons 2nd law now has been cast in the form:

$$M\frac{d^2\boldsymbol{R}}{dt^2} = \boldsymbol{F}^{\text{ext}}. \tag{1.10}$$

Physically, this means that the center of mass of the many-particle system moves as if all the mass was concentrated in the CM position. Moreover, since the total momentum is

$$\boldsymbol{P} = \sum m_i \frac{d\boldsymbol{r}_i}{dt} = M\frac{d\boldsymbol{R}}{dt}, \tag{1.11}$$

we see that if the total external force $\boldsymbol{F}^{\text{ext}}$ is zero, then the total momentum $\boldsymbol{P}$ is conserved. This is called the *weak* law of action and reaction.

The same line of reasoning may be applied to the total angular momentum $\boldsymbol{L} = \sum_i \boldsymbol{r}_i \times \boldsymbol{p}_i$ of the system. Performing a differentiation with respect to time and inserting equation (1.7) into this equation, we obtain

$$\dot{\boldsymbol{L}} = \sum_i \boldsymbol{r}_i \times \boldsymbol{F}_i^{\text{ext}} + \sum_{\substack{i,j \\ i \neq j}} \boldsymbol{r}_i \times \boldsymbol{F}_{ji}. \tag{1.12}$$

The last term can be written as a summation over pairs of the form:

$$\boldsymbol{r}_i \times \boldsymbol{F}_{ji} + \boldsymbol{r}_j \times \boldsymbol{F}_{ij} = (\boldsymbol{r}_i - \boldsymbol{r}_j) \times \boldsymbol{F}_{ji}, \tag{1.13}$$

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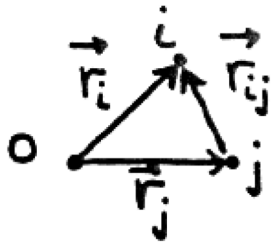
where we used that $\boldsymbol{F}_{ij} = -\boldsymbol{F}_{ji}$. Defining $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, we may then write

$$\dot{\boldsymbol{L}} = \boldsymbol{\tau}^{\text{ext}} + \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \boldsymbol{r}_{ij} \times \boldsymbol{F}_{ji}. \tag{1.14}$$



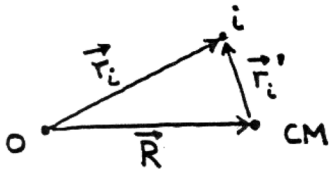
The benefit of doing so is clear by inspecting the last term: if the force between particles i and j lies along the line which connects i and j - this is the *strong* law of action and reaction - then $\boldsymbol{r}_{ij} \times \boldsymbol{F}_{ji} = 0$ for all i and j. We end up with:

$$\dot{\boldsymbol{L}} = \boldsymbol{\tau}^{\text{ext}}. \tag{1.15}$$

We see that in the same way as for the total linear momentum, the total angular momentum $\boldsymbol{L}$ for a system of many particles is conserved if the net external torque $\boldsymbol{\tau}^{\text{ext}}$ is zero. We emphasize that it was crucial for this derivation that the forces were *central*, meaning that forces act along the line connecting any pair of particles.

It is also instructive to rewrite the total angular momentum $\boldsymbol{L}$ in a slightly different way, which brings out the contribution to $\boldsymbol{L}$ both from the CM motion and the relative motion around the CM. The coordinate vector to any particle i may be written as $\boldsymbol{r}_i = \boldsymbol{R} + \boldsymbol{r}_i^{'}$ where $\boldsymbol{r}_i^{'}$ represents the distance from the CM to particle i. In the same way, $\boldsymbol{v}_i = \boldsymbol{V} + \boldsymbol{v}_i^{'}$. We obtain:

$$\boldsymbol{L} = \sum_i \boldsymbol{r}_i \times \boldsymbol{p}_i = \sum_i \boldsymbol{R} \times m_i \boldsymbol{V} + \sum_i \boldsymbol{r}_i^{'} \times m_i \boldsymbol{v}_i^{'} + (\sum_i m_i \boldsymbol{r}_i^{'}) \times \boldsymbol{V} + \boldsymbol{R} \times \frac{d}{dt}(\sum_i m_i \boldsymbol{r}_i^{'}). \tag{1.16}$$



By considering the definition of the CM position $\boldsymbol{R}$ and the relative coordinate $\boldsymbol{r}_i^{'}$, one finds that $(\sum_i m_i \boldsymbol{r}_i^{'}) = 0$. Thus, the two last terms in the above equation vanish and we are left with

$$\boldsymbol{L} = \boldsymbol{R} \times M\boldsymbol{V} + \sum_i \boldsymbol{r}_i^{'} \times \boldsymbol{p}_i^{'}. \tag{1.17}$$

In other words, the total angular momentum around the origo is equal to the angular momentum of an object positioned in the CM with the total mass M of the system *plus* the angular momentum around the CM itself. We see that if the CM is stationary, $\boldsymbol{R}$ is constant and thus $\boldsymbol{V} = 0$, meaning that $\boldsymbol{L}$ is equal to the angular momentum around the CM.

The contribution to the kinetic energy of a many-particle system can also be split up in the same way: a part pertaining to the motion of the CM and a part pertaining to the relative motion around the CM. We obtain:

$$T = \frac{1}{2} \sum_i m_i \boldsymbol{v}_i^2 = \frac{1}{2} \sum_i m_i (\boldsymbol{V} + \boldsymbol{v}_i^{'})(\boldsymbol{V} + \boldsymbol{v}_i^{'}) = \frac{1}{2} M \boldsymbol{V}^2 + \frac{1}{2} \sum_i m_i (\boldsymbol{v}_i^{'})^2. \tag{1.18}$$

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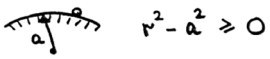
C. Constraints and generalized coordinates

Particles moving around in a system may be subject to constraints. Examples of this would include a gas in a container, where the particles cannot have positions $\boldsymbol{r}_i$ outside of the container, or a ball rolling down a hill, with the criterium that the ball must always touch the ground. Various constraints can be classified in different ways:

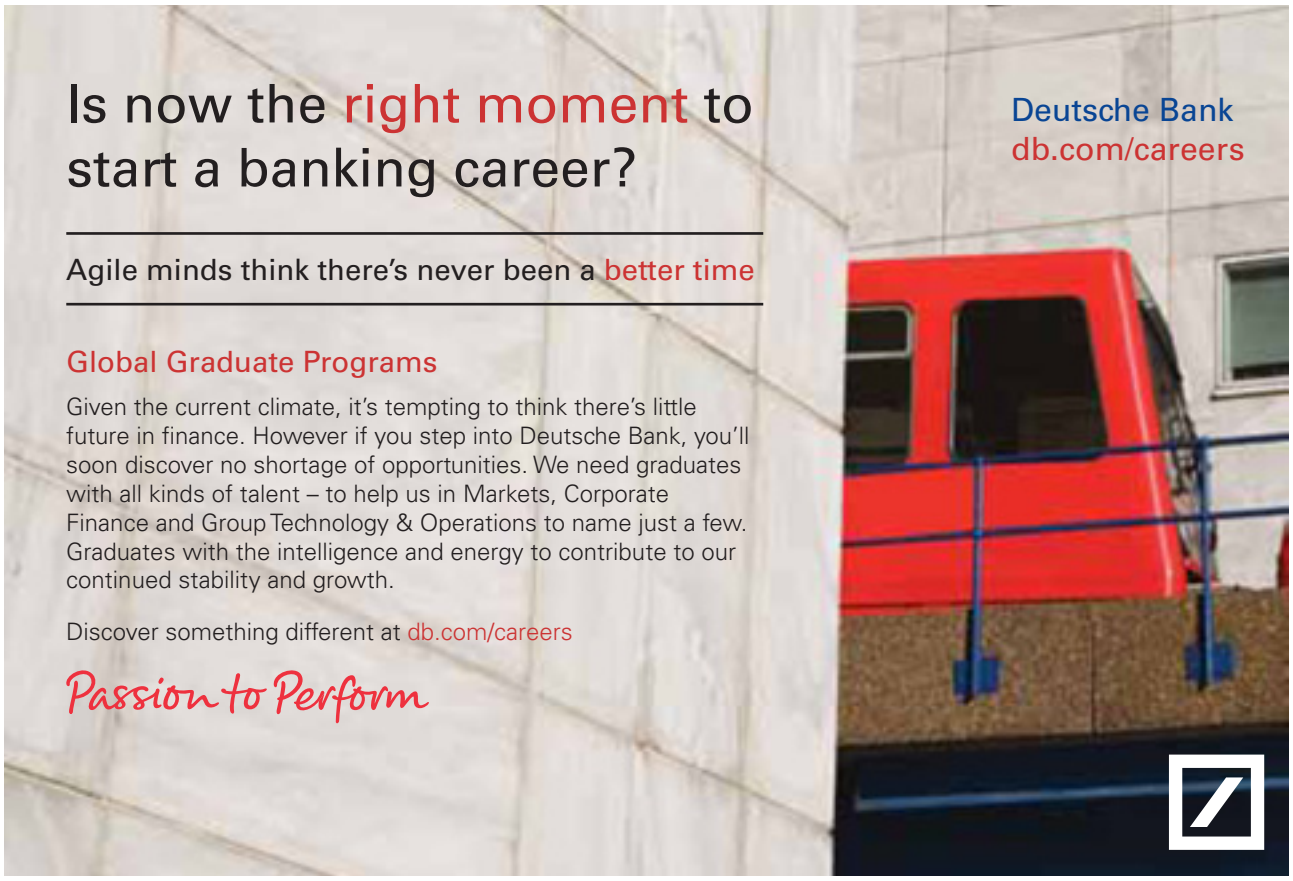
Holonomic constraints: May be written as $f(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, t) = 0$. An example is the equation for a rigid body (the distance between two points is constant): $(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 - c_{ij}^2 = 0$.

Non-holonomic constraints: May not be expressed in the form $f(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, t) = 0$. An example is a person running on a hill: his or her position may be on the ground or above the ground, but not inside the hill. If the radius of the hill is a, we thus have the constraint $r^2 - a^2 \geq 0$.



One also speaks of rheonomous constraints which are time-dependent, and scleronomous constraints which are time-independent. Having introduced constraints leads us to the important concept of generalized coordinates. Imagine that we have a system with N particles that can move in all three dimensions. We would then say that we have $3N$ degrees of freedom: each particle can move in three different directions, with each one corresponding to a degree of freedom in the particle's motion. If there are k holonomic restrictions present in the system, the number of degrees of freedom will be reduced. Where there were originally $3N$ degrees of freedom, there are now $3N - k$.

To put this mathematically, let $\boldsymbol{r}_i$ denote the position vector of each of the N particles. However, not all of these position vectors can be independent since there are constraints in the system: for instance, the distance between two particles is fixed for a rigid body. Thus, there are instead $3N - k$ independent coordinates which we name $q_1, q_2, \ldots q_{3N-k}$. These *generalized coordinates* thus take into account the constraints of the system and can be used to describe the position vectors $\boldsymbol{r}_i$. We have: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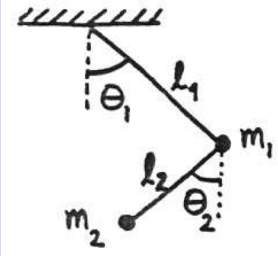
$$\begin{aligned} \boldsymbol{r}_1 &= \boldsymbol{r}_1(q_1, q_2, \ldots q_{3N-k}, t), \\ \boldsymbol{r}_2 &= \boldsymbol{r}_2(q_1, q_2, \ldots q_{3N-k}, t), \\ &\vdots \\ \boldsymbol{r}_N &= \boldsymbol{r}_N(q_1, q_2, \ldots q_{3N-k}, t), \end{aligned} \tag{1.19}$$

(1.20)

Example 1. Double-pendulum moving in a plane. With two particles, we would expect to have 6 degrees of freedom. However, restricting the motion of the pendulum to take place in a plane, i.e. moving in 2D rather than 3D, we are removing one degree of freedom per particle. We are then left with 4 degrees of freedom. When we additionally demand that the distance between the particles is constant, for instance having the particles connected by a rigid rod, we are removing one more degree of freedom per particle. We thus end up with a total of 6-4=2 degrees of freedom. These 2 degrees of freedom are the generalized coordinates. For our particular system under consideration, the generalized coordinates are θ_1 and θ_2 in the figure.



D. D'Alembert's principle and Lagrange's equations

As a preliminary to this section, we first define the concept of a *virtual displacement*: it is an infinitesimal displacement $\delta\boldsymbol{r}_i$ of the coordinates of the system which respects any constraints that are present. Assume first that we're dealing with a system in equilibrium. This means that all forces acting on particles is equal to zero, $\boldsymbol{F}_i = 0$. As a result, we also have $\sum_i \boldsymbol{F}_i \cdot \delta\boldsymbol{r}_i = 0$. Now, the force acting on particle i can be split up into an externally applied force $\boldsymbol{F}_i^a$ and a force $\boldsymbol{f}_i$ resulting from constraints in the system:

$$\boldsymbol{F}_i = \boldsymbol{F}_i^a + \boldsymbol{f}_i. \tag{1.21}$$

An example of a constraint force would be the force exerted by the wall on a particle inside a gas container. It is reasonable to assume that $\boldsymbol{f}_i \cdot \delta\boldsymbol{r}_i = 0$: any force constraining the motion of a particle i should act perpendicularly to any allowed displacement $\delta\boldsymbol{r}_i$. Another way to put this is to say that forces from constraints do no work. We can see this *e.g.* for the normal-force from the floor acting on objects on it. When this force acts, the object is only allowed to be displaced perpendicularly to it (along the floor). It is important to note that we are excluding friction in this way, which would not satisfy $\boldsymbol{f}_i \cdot \delta\boldsymbol{r}_i = 0$. However, we shall return to see how friction may be incorporated later on. We are now left with

$$\sum_i \boldsymbol{F}_i^a \cdot \delta\boldsymbol{r}_i = 0. \tag{1.22}$$

Note that this equation does not imply that each $\boldsymbol{F}_i^a$ is zero, since the $\delta\boldsymbol{r}_i$ vectors are not independent in general because of the presence of constraints. Only if we use generalized coordinates, which as we have seen take into account the presence of constraints, can we say that the coordinates are independent on each other.

Let us now turn to the more interesting case of a system in motion, in effect out of equilibrium. The equation of motion for particle i is then given by Newton's 2nd law, $\boldsymbol{F}_i - \dot{\boldsymbol{p}}_i = 0$. Analogously with the static case above, we may decompose the force into an applied part and a part due to constraints. Performing a summation over i and taking the scalar product with the virtual displacement, we obtain:

$$\sum_i (\boldsymbol{F}_i^a - \dot{\boldsymbol{p}}_i) \cdot \delta\boldsymbol{r}_i = 0. \tag{1.23}$$

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This is called D'Alembert's principle and the merit of this equation is that we have now eliminated the forces stemming from constraints in the system. By assuming (without much loss of generality) that the constraints are holonomic, we may introduce generalized coordinates as described earlier:

$$\boldsymbol{r}_i = \boldsymbol{r}_i(q_1, q_2, \dots q_n, t). \tag{1.24}$$

It follows that the velocity of particle i is given by (via the chain rule):

$$\boldsymbol{v}_i = \dot{\boldsymbol{r}}_i = \sum_i \frac{\partial \boldsymbol{r}_i}{\partial q_i}\dot{q}_i + \frac{\partial \boldsymbol{r}_i}{\partial t} = \boldsymbol{v}_i(q_i, \dot{q}_i, t). \tag{1.25}$$

Similarly, the virtual displacement $\delta\boldsymbol{r}_i$ of the position vector itself may be written in terms of the virtual displacement of the generalized coordinates:

$$\delta\boldsymbol{r}_i = \sum_j \frac{\partial \boldsymbol{r}_i}{\partial q_j}\delta q_j. \tag{1.26}$$

Note that virtual displacements involve only coordinate-displacements and not time, so that δt does not enter: the displacement takes place at a fixed time. Let us now examine D'Alembert's principle in more detail to see what comes out of it. The first term is:

$$\sum_i \boldsymbol{F}_i \cdot \delta\boldsymbol{r}_i = \sum_{i,j} \boldsymbol{F}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j}\delta q_j \equiv \sum_j Q_j \delta q_j. \tag{1.27}$$

We defined the *generalized force* $Q_j = \sum_i \boldsymbol{F}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j}$. Note that the dimension of $Q_j\delta q_j$ is work. The dimensions of Q_j and δq_j themselves will however depend on the geometry. For instance, if q_j denotes an angle with dimension rad, the dimension of Q_j will be J/rad.

We now look at the second term of D'Alembert's principle.

$$\sum_i \dot{\boldsymbol{p}}_i \cdot \delta\boldsymbol{r}_i = \sum_{i,j} m_i \ddot{r}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j}\delta q_j. \tag{1.28}$$

We can rewrite as follows:

$$\sum_i m_i \ddot{\boldsymbol{r}}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} = \sum_i \Big[\frac{d}{dt}(m_i \dot{\boldsymbol{r}}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j}) - m_i \dot{\boldsymbol{r}}_i \frac{d}{dt}\frac{\partial \boldsymbol{r}_i}{\partial q_j}\Big] \tag{1.29}$$

In the last term in the above equation, we may exchange the order of $\frac{d}{dt}$ and $\frac{\partial}{\partial q_j}$:

$$\frac{d}{dt}\frac{\partial \boldsymbol{r}_i}{\partial q_j} = \frac{\partial}{\partial q_j}\frac{d\boldsymbol{r}_i}{dt}. \tag{1.30}$$

To see why this is allowed, we look at how these operators act on $\boldsymbol{r}_i$ in detail. If we first differentiate with respect to q_j and then with respect to time, we get:

$$\frac{d}{dt}\frac{\partial \boldsymbol{r}_i}{\partial q_j} = \sum_k \frac{\partial^2 \boldsymbol{r}_i}{\partial q_j \partial q_k}\dot{q}_k + \frac{\partial^2 \boldsymbol{r}_i}{\partial q_j \partial t}. \tag{1.31}$$

Now reverse the order: differentiate with respect to time first and then with respect to q_j to obtain

$$\frac{\partial}{\partial q_j}\frac{d\boldsymbol{r}_i}{dt} = \frac{\partial}{\partial q_j}\boldsymbol{v}_i = \frac{\partial}{\partial q_j}\Big(\sum_k \frac{\partial \boldsymbol{r}_i}{\partial q_k}\dot{q}_k + \frac{\partial \boldsymbol{r}_i}{\partial t}\Big). \tag{1.32}$$

The result is seen to be identical. In the same way, one can also show that

$$\frac{\partial \boldsymbol{v}_i}{\partial \dot{q}_j} = \frac{\partial \boldsymbol{r}_i}{\partial q_j}. \tag{1.33}$$

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Using the above relations in equation (1.29), we get:

$$\begin{aligned}\sum_i m_i \ddot{\boldsymbol{r}}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} &= \sum_i \left[\frac{d}{dt}(m_i \boldsymbol{v}_i \cdot \frac{\partial \boldsymbol{v}_i}{\partial \dot{q}_j}) - m_i \boldsymbol{v}_i \cdot \frac{\partial \boldsymbol{v}_i}{\partial q_j}\right] \\ &= \sum_i \left[\frac{d}{dt}\frac{\partial}{\partial \dot{q}_j}(\frac{1}{2} m_i v_i^2) - \frac{\partial}{\partial q_j}(\frac{1}{2} m_i v_i^2)\right] \\ &= \frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j}. \end{aligned} \tag{1.34}$$

We may then rewrite D'Alembert's principle in the following way:

$$\sum_j \left[\frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} - Q_j\right]\delta q_j = 0. \tag{1.35}$$

Actually, we can make an even stronger statement: each term inside the summation has to be zero individually. The key to making this statement is to realize that with holonomic constraints, which we assumed, all generalized coordinates are independent of each other. Thus, δq_j are independent quantities and the following n second order equations must be satisfied:

$$\frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} = Q_j. \tag{1.36}$$

Let us make one more assumption, which still includes a vast number of physical situations, and set our system to be conservative: $\boldsymbol{F}_i = -\nabla_i V$, with $V = V(q_j)$. We then get for the generalized force, using the chain rule,

$$Q_j = \sum_i \boldsymbol{F}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} = -\sum_i \nabla_i V \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} = -\frac{\partial V}{\partial q_j}. \tag{1.37}$$

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The potential V depends on the coordinates, but not on the generalized velocities $\dot{q}_i$. We will later see how to deal with velocity-dependent potentials. In that case, we may add a term to equation (1.36) which is equal to zero, namely $\partial V/\partial\dot{q}_j$. We have thus ended up with

$$\boxed{\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0,}$$

where we defined the Lagrange function $L = T - V$. *These are the Lagrange equations:* arguably the most important equations in this entire book. They were derived under the assumption of a holonomic and conservative system. There are in general n Lagrange equations, each of second order. We thus need $2n$ initial conditions in all.

An important feature to notice is that L is in fact not uniquely defined. The physics is *unchanged* if we instead of L use L' where $L' = L + \frac{dF(q,t)}{dt}$ as can be verified by direct insertion. The Lagrange equations remain the same, as we will now see an example of in the last subsection of this chapter.

Note that in deriving the Lagrange equations, we have ended up with simpler equations that involve *scalar functions*, the kinetic energy T and potential energy V, rather than working with vectors such as the force $\boldsymbol{F}_i$ and acceleration $\boldsymbol{a}_i$ for each particle. Moreover, we have automatically included the role played by constraints in the system since it is the generalized coordinates q_i that enter the Lagrange equations.

E. Levi-Civita symbol

Before proceeding to discuss extensions and modifications of the Lagrange equations, it is useful here to introduce the mathematical quantity known as the Levi-Civita tensor ϵ_{ijk}. To see how this works, we also introduce some convenient notation for working with vectors. Using Cartesian coordinates, we write

$$\boldsymbol{A}\cdot\boldsymbol{B} = \sum_i A_i B_i \equiv A_i B_i, \tag{1.38}$$

which is known as a sum convention: repeated indices implies summation over them. We may then also write:

$$\nabla\cdot\boldsymbol{A} = \frac{\partial A_i}{\partial x_i} = \partial_i A_i \tag{1.39}$$

and

$$\nabla\phi = \boldsymbol{e}_i\partial_i\phi, \tag{1.40}$$

where $\boldsymbol{e}_i$ is the unit vector in i direction. As for the Levi-Civita symbol, it is antisymmetric in all indices and changes sign when two indices exchange position. Moreover, it is equal to zero when at least two indices are the same. Thus, we have that

$$\begin{aligned}\epsilon_{ijk} &= +1 \text{ when } i,j,k \text{ are exchanged in a cyclic manner}(\varepsilon_{123} = +1),\\ \epsilon_{ijk} &= -1 \text{ when } i,j,k \text{ are exchanged in an anticyclic manner}(\varepsilon_{132} - 1),\end{aligned} \tag{1.41}$$

This notation is particularly useful when dealing with cross-products. If $\boldsymbol{A} = \boldsymbol{B}\times\boldsymbol{C}$, then $A_i = \epsilon_{ijk}B_jC_k$. Since j and k are repeated indices, a summation over both is implied. It is also handy to note the relation

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}. \tag{1.42}$$

Example 2. Using the Levi-Civita tensor.

$$\begin{aligned}(\boldsymbol{A}\times\boldsymbol{B})\cdot(\boldsymbol{C}\times\boldsymbol{D}) &= (\boldsymbol{A}\times\boldsymbol{B})_i(\boldsymbol{C}\times\boldsymbol{D})_i = \varepsilon_{ijk}A_jB_k\epsilon_{ilm}C_lD_m\\ &= (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl})A_jB_kC_lD_m = (\boldsymbol{A}\cdot\boldsymbol{C})(\boldsymbol{B}\cdot\boldsymbol{D}) - (\boldsymbol{A}\cdot\boldsymbol{D})(\boldsymbol{B}\cdot\boldsymbol{C}).\end{aligned} \tag{1.43}$$

Note that quantities such as $\varepsilon_{ijk}, A_j, B_k$ are scalar which means that they can be moved around as we please (scalars commute).

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F. Friction and other velocity-dependent potentials

Armed with the Levi-Civita tensor, we now pose the question: what happens with Lagrange's equations if the potential depends on velocity? The answer is that Lagrange's equations keep their form if $L = T - U$ and $Q_j = -\frac{\partial U}{\partial q_j} + \frac{d}{dt}\frac{\partial U}{\partial \dot{q}_j}$ where $U = U(q_j, \dot{q}_j)$ is the velocity-dependent potential. Here q_j and $\dot{q}_j$ are regarded as independent variables.
An important example of this is the electromagnetic potential. From electrodynamics, we know that the Lorentz-force is the force acting on a particle with charge q moving in an electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ field with velocity $\boldsymbol{v}$:

$$\boldsymbol{F} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}). \tag{1.44}$$

The electric and magnetic fields themselves can be written in terms of a vector potential $\boldsymbol{A}$ and a scalar potential ϕ. This can be seen by considering two of Maxwell's equations:

$$\nabla \cdot \boldsymbol{B} = 0,\ \nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}. \tag{1.45}$$

The first of these equations shows that we can always write $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ since the divergence of a curl is zero. Inserting this into the second equation, we obtain

$$\nabla \times (\boldsymbol{E} + \frac{\partial \boldsymbol{A}}{\partial t}) = 0. \tag{1.46}$$

Since the curl of a divergence is also zero, it follows that we can write $\boldsymbol{E} + \frac{\partial \boldsymbol{A}}{\partial t} = -\nabla\phi$. We can now express the Lorentz-force in terms of $\boldsymbol{A}$ and ϕ instead of $\boldsymbol{E}$ and $\boldsymbol{B}$:

$$\boldsymbol{F} = q(-\nabla\phi - \frac{\partial \boldsymbol{A}}{\partial t} + \boldsymbol{v} \times \nabla \times \boldsymbol{A}). \tag{1.47}$$

You may wonder why we would like to replace the electric and magnetic fields with the vector potential and the scalar field. What is the benefit of this? This is related to a concept known as *gauge-invariance* which we shall return to later on in the chapter on the special theory of relativity.

To continue working with the Lorentz-force, it is convenient at this point to make use of the Levi-Civita symbol. By using that

$$[\boldsymbol{v} \times (\nabla \times \boldsymbol{A})]_i = v_j \partial_i A_j - v_j \partial_j A_i, \tag{1.48}$$

we get:

$$F_i = q(-\partial_i \phi - \partial_t A_i + v_j \partial_i A_j - v_j \partial_j A_i). \tag{1.49}$$

Note that ∂_i and A_j do *not* commute, since ∂_i is an operator acting on whatever comes after it. On the other hand, ∂_i and v_j do commute since the velocity v_j has no explicit dependence on position (it is, as we know, defined as the derivative of position with respect to time). It follows that the relations below hold:

$$\begin{aligned} v_j \partial_i A_j &= \partial_i (\boldsymbol{v} \cdot \boldsymbol{A}), \\ \frac{dA_i}{dt} &= \frac{\partial A_i}{\partial t} + v_j \partial_j A_i, \end{aligned} \tag{1.50}$$

and thus we can rewrite equation (1.49) as

$$\begin{aligned} F_i &= q[-\partial_i \phi + \partial_i (\boldsymbol{v} \cdot \boldsymbol{A}) - \frac{dA_i}{dt}] \\ &= q[-\partial_i (\phi - \boldsymbol{v} \cdot \boldsymbol{A}) - \frac{d}{dt}\frac{\partial}{\partial v_i}(\boldsymbol{A} \cdot \boldsymbol{v})] \\ &= -\partial_i U + \frac{d}{dt}\frac{\partial U}{\partial v_i} \end{aligned} \tag{1.51}$$

where we defined $U = q\phi - q\boldsymbol{A} \cdot \boldsymbol{v} = U(\boldsymbol{r}, \boldsymbol{v})$. Note that in the second term we have made use of the fact that ϕ is a function of $\mathbf{r}$ and t only; thus $\partial\phi/\partial v_i = 0$.

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We have managed to write the force on a form which is consistent with the Lagrange equations in the form we derived in the previous section, and we thus identify U as the generalized velocity-dependent potential. The Lagrange function is then:

$$L = T - U = T - q\phi + q\boldsymbol{A} \cdot \boldsymbol{v}. \tag{1.52}$$

This is called minimal coupling in field theory. We emphasize that U is *not* the potential energy of the particle, unlike the case we considered previously where the potential energy only depended on position. In fact, it is instructive to consider in some more detail whether or not the electromagnetic force is conservative or not.

We know from its definition that a conservative force can be written as the gradient of a scalar potential, and ensures that energy $T + V$ is conserved. If we only have a pure electric field, we see that the Lorentz-force can indeed be written as the gradient of a scalar potential since $\boldsymbol{E} = -\nabla\phi$. A purely electric force is thus conservative. But what if we also have a magnetic field? In this case, it is clear that the Lorentz-force *cannot* be written as the gradient of a scalar potential. Hence, magnetic forces are formally classified as non-conservative. What is the implication with respect to energy conservation? Well, we know that magnetic forces do no work since the force acts perpendicularly to the velocity (due to the cross-product between velocity and magnetic field). So while the magnetic force is formally classified as non-conservative, as it cannot be written as the gradient of a scalar potential, that does not necessarily mean that energy is not conserved. For instance, energy is stored in the electromagnetic field itself which thus in principle can be converted into mechanical energy for a charged particle.

In general, to calculate the magnetic field energy built up when a magnetic field is being applied, we must examine the *electric* fields induced by the change in the magnetic field and determine the work done by these fields on the currents producing the magnetic field. The electric field here is in a sense a second, though indispensable, ingredient. The total energy, however, has to be conserved. We will later derive the fundamental result that the exact criterium for energy to be conserved is that there is no explicit time-dependence in the Lagrange function L. So as long as the functions ϕ and $\boldsymbol{A}$ are time-independent, energy is conserved even if the magnetic force is said to be non-conservative.

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Another important non-conservative force is **friction**. For a holonomic system, Lagrange's equations may always be written in the form:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = Q_i \tag{1.53}$$

where L contains the potential from conservative forces while Q_i contains the forces that *cannot* be derived from a potential. Frictional forces are an example of this. The origin of friction is actually electromagnetic in nature, but frictional forces may often be well accounted for by a phenomenological form: namely, by setting the frictional force $\boldsymbol{F}_f$ to be proportional to the velocity $\boldsymbol{v}$ of the particle. For one particle moving along the x axis, we thus have

$$F_{f,x} = -k_x v_x = -\frac{\partial}{\partial v_x}(\frac{1}{2}k_x v_x^2). \tag{1.54}$$

The work performed by the system to overcome the frictional force can be computed as follows:

$$dW_f = -\boldsymbol{F}_f \cdot d\boldsymbol{r} = -\boldsymbol{F}_f \cdot \boldsymbol{v}dt = (k_x v_x^2 + k_y v_y^2 + k_z v_z^2)dt. \tag{1.55}$$

For several particles moving in three dimensions, $\boldsymbol{F}_f = -\nabla_v \mathcal{F}$. Here, we have introduced Rayleigh's dissipation function $\mathcal{F} = \frac{1}{2}\sum_i (k_x v_{ix}^2 + k_y v_{iy}^2 + k_z v_{iz}^2)$ where the subscript i denotes particle i. We see that we can then express the rate of energy loss due to friction via the dissipation function: it is simply $dW_f/dt = 2\mathcal{F}$. The generalized force stemming from friction may be computed by going back to the definition of generalized forces:

$$Q_j = \sum_i \boldsymbol{F}_{i,f} \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} = -\sum_i \nabla_{v_i}\mathcal{F} \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} = -\sum_i \nabla_{v_i}\mathcal{F} \cdot \frac{\partial \dot{\boldsymbol{r}}_i}{\partial \dot{q}_j} = -\frac{\partial \mathcal{F}}{\partial \dot{q}_j}. \tag{1.56}$$

Lagrange's equations now read:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} + \frac{\partial \mathcal{F}}{\partial \dot{q}_i} = 0. \tag{1.57}$$

In other words, we need to know two scalar functions L and $\mathcal{F}$ in order to obtain the equations of motion for a system with friction.

The case where $\boldsymbol{F}_f$ is proportional to $\boldsymbol{v}$ is actually of great importance in physics, especially in microfuidics and in medical technology. It ought to be emphasized, however, that the equation is applicable only under the condition that the velocity v is "small" when looked upon in conjunction with the viscosity of the fluid through which the body is moving. Explicitly, the condition is that the so-called Reynolds number Re must be much less than one. The definition of the Reynolds number is $Re = \rho v l/\mu$, where ρ is the density of the surrounding fluid, l a typical length, and μ the dynamic viscosity. For a sphere of radius R, for instance, one can simply put $l = 2R$. As an example, consider a human cell for which approximately $R = 5$ μm, traveling at a speed not greater than 10 μm/s. Then Re is of order 10^{-4}, showing that the above condition is amply satisfied and that viscous forces are dominant.

Another case is a DNA molecule, which can be stretched into a linear strand by hydrodynamical means. Imagine that one end of the DNA is attached to a glass plate and that a spherical bead is fixed to the other end, giving hydrodynamic drag to a viscous liquid flowing past, parallel to the plate. In this way the DNA becomes stretched. Increasing the fluid velocity until the strand snaps, one can actually determine the elastic strength of the strand.

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G. Examples

In this subsection, we want to look at the Lagrange equations "in action" and so we consider several examples that illustrate their usage.

Example 3. One particle with Cartesian coordinates. Before proceeding to derive the Lagrange equations for this system, which effectively constitute the equations of motion describing the particle, take a moment to think about what you would expect that the equations look like. That's right - we should expect to recover Newtons 2nd law for a particle moving under influence of a force. For our system, we have $T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$. It follows that:

$$\begin{aligned} &\frac{\partial T}{\partial x} = \frac{\partial T}{\partial x} = \frac{\partial T}{\partial x} = 0, \\ &\frac{\partial T}{\partial x} = m\dot{x}, \ \frac{\partial T}{\partial y} = m\dot{y}, \ \frac{\partial T}{\partial y} = m\dot{y}. \end{aligned} \tag{1.58}$$

The equation of motion is:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = Q_i \tag{1.59}$$

where $q_1 = x, q_2 = y, q_3 = z$ and $Q_i = F_i$. The equations of motion become

$$\frac{d}{dt}(m\dot{x}) = F_x \tag{1.60}$$

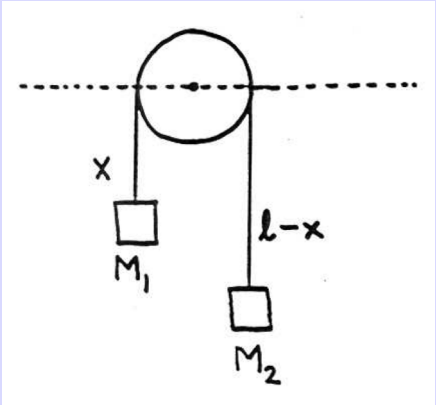
and identical for y and z, meaning that we as expected recovered Newton's 2nd law.

Example 4. Atwood's machine. There is only one independent (generalized) coordinate, namely x. To construct the Lagrange equations, we first need to identify the Lagrange function L. To do so, we need the potential energy V and kinetic energy T.

$$\begin{aligned} V &= -M_1 g x - M_2 g(l - x), \\ T &= \frac{1}{2}(M_1 + M_2)\dot{x}^2, \\ L &= T - V = \frac{1}{2}(M_1 + M_2)\dot{x}^2 + M_1 g x + M_2 g(l - x). \end{aligned} \tag{1.61}$$

The Lagrange equation for x then becomes:

$$(M_1 + M_2)\ddot{x} = (M_1 - M_2)g. \tag{1.62}$$



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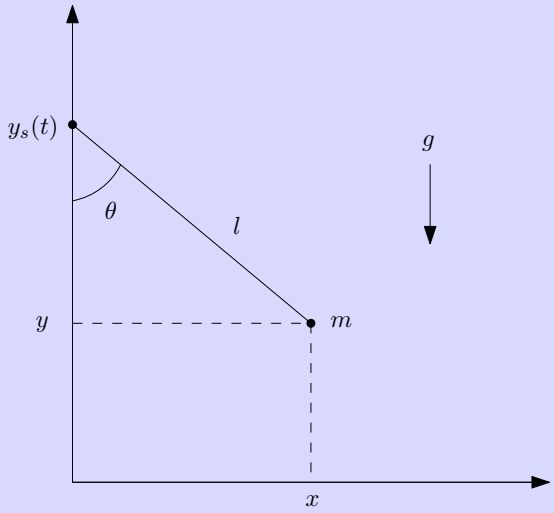
Example 5. Pendulum driven at the pivot. This example is a slightly modified version of the one found in "Structure and Interpretation of Classical Mechanics" section 1.6.2 by Gerald Sussman and Jack Wisdom. We previously stated that the Lagrange function is not uniquely defined: we could add a total derivative of a function, $dF(q,t)/dt$, to L without changing the equations of motion. To see how this fact can be used to one's advantage, consider the system shown in the figure: a pendulum driven by vertical motion of the pivot $\mathcal{P}$ which slides along the y-axis. The pendulum itself is taken to be a point mass m which gravity acts upon. Since the pivot is driven, for instance by some engine or by hand, its vertical position is a given function of time $y_s(t)$.



In order to construct the Lagrange function, we first need to establish what the generalized coordinates are. The mass m can

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move in the 2D plane, which naively might suggest that there are 2 degrees of freedom. In reality, however, there is only one because the length l of the rod is fixed. Thus, the only degree of freedom is the angle θ and this is our generalized coordinate. The position of m can then be written as

$$x = l\sin\theta \text{ and } y = y_s(t) - l\cos\theta. \tag{1.63}$$

The corresponding velocities are

$$v_x = l\dot{\theta}\cos\theta,\ v_y = \dot{y}_s(t) + l\dot{\theta}\sin\theta. \tag{1.64}$$

We can now write down the kinetic energy T as

$$T = \frac{1}{2}m(v_x^2 + v_y^2) = \frac{1}{2}m[l^2\dot{\theta}^2 + (\dot{y}_s)^2 + 2l\dot{y}_s\dot{\theta}\sin\theta]. \tag{1.65}$$

The potential energy is $V = mgy = mg(y_s - l\cos\theta)$. The Lagrange equation may now be obtained by using $L = T - V$:

$$\ddot{\theta}l^2m + ml(\ddot{y}_s + g)\sin\theta = 0. \tag{1.66}$$

Here's a tip: whenever you derive an equation, pause for a moment and consider it to see if it makes physical sense. What is the above equation telling us?

When deriving an equation, it is often useful to check limiting cases in order to see if we recover a physically sensible result.

By inspecting the above equation, we see that an interesting interpretation emerges: the equation of motion is identical to that of an undriven pendulum except that gravity g has been replaced by $g + \ddot{y}_s$. This means that the effective acceleration of the mass is gravity augmented by the acceleration of the pivot itself. This is physically sensible. However, we probably could not have guessed that this would be the case just by looking at the Lagrange function. This is where the power of the non-uniqueness of the Lagrange function comes into play. Namely, by writing an alternative Lagrangian which has the same equations of motion, but which is much easier to interpret than the original Lagrange function. Consider thus the following Lagrange function

$$L'(\theta, \dot{\theta}, t) = \frac{1}{2}ml^2\dot{\theta}^2 + ml(g + \ddot{y}_s)\cos\theta. \tag{1.67}$$

With this Lagrange function, it is immediately clear that the accelerating pivot has the net effect that it modifies the acceleration due to gravity. The equation of motion obtained from this Lagrange function is identical to equation (1.66), and hence both L and L' give exactly the same physics. For this to be the case, we then know we should to be able to write the difference between L' and L as a total time derivative. The difference between the two is:

$$\Delta L = L - L' = \frac{1}{2}m\dot{y}_s^2 + ml\dot{y}_s\dot{\theta}\sin\theta - gmy_s - ml\ddot{y}_s\cos\theta. \tag{1.68}$$

There are four terms. Two of these terms are independent on both θ and $\dot{\theta}$. This means that they act as constants with regard to the Lagrange equation and thus have no effect. They can simply be discarded: one can always add an arbitrary constant to a Lagrange function without changing the physics (think of this as redefining the potential energy minimum). Now, the two other terms can indeed be rewritten as a total time derivative:

$$+ml\dot{y}_s\dot{\theta}\sin\theta - ml\ddot{y}_s\cos\theta = \frac{dF(t,\theta)}{dt} \text{ where } F(t,\theta) = -ml\dot{y}_s\cos\theta. \tag{1.69}$$

We have thus established both mathematically and by physical intuition why the two Lagrangians give the same result.

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II. LAGRANGE'S EQUATIONS AND THE VARIATIONAL PRINCIPLE

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Learning goals. After reading this chapter, the student should:

- Understand the foundation of the variational principle and be able to use it in practical calculations
- Know how to include non-holonomic constraints in Lagrange's equations
- Understand the close relation between symmetries and conservation laws

A. Hamilton's principle

In the previous chapter, we derived Lagrange's equations from a differential principle (D'Alemberts principle) by considering small virtual displacements from a given state. In this chapter we instead derive Lagrange's equations from an *integral* principle. What this means is that we will consider variations in the motion of the entire system between two times t_1 and t_2.

Let us clarify what is really meant by the "motion of the entire system". We define the configuration space as spanned by the axes of the n generalized coordinates $\{q_1, q_2, q_n\}$ ($n = 3N - k$). The position or *state* of the system is at any time t given by one point in this configuration space. The motion of the system is thus described by a curve in configuration space where each point on the curve represents the entire system's configuration at a specific time. One advantage of using Hamilton's principle is that we are deriving the dynamics of the system from an expression which depends on the motion of the entire system between times t_1 and t_2. This makes it convenient to generalize it to quantum mechanics since in this formulation all possible paths the system can take contribute.

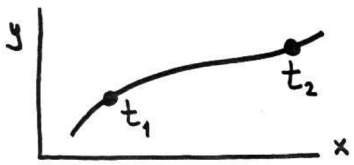
We now define mathematically what Hamilton's principle means. The system will move from time t_1 to t_2 such that *the action* I defined as

$$I = \int_{t_1}^{t_2} L dt \tag{2.1}$$

has a stationary value (also known as extremal value). Here, $L = L(q, \dot{q}, t) = T - V$ is the Lagrange function and we have a conservative system if $V = V(q)$. Hamilton's principle is also valid more generally if $V \to U = U(q, \dot{q}, t)$. Systems described by either U or V are called monogenic. Hamilton's principle may also be expressed as follows:

$$\delta I = \delta \int_{t_1}^{t_2} L(q_1 \dots q_n, \dot{q}_1 \dots \dot{q}_n, t) dt = 0, \tag{2.2}$$

and we shall see that Lagrange's equations follow from Hamilton's principle.



B. Derivation of Lagrange's equations from Hamilton's principle

Assume for simplicity that we just have one degree of freedom $q = q(t)$. The proof below is straight forward to generalize to multiple degrees of freedom q_i.

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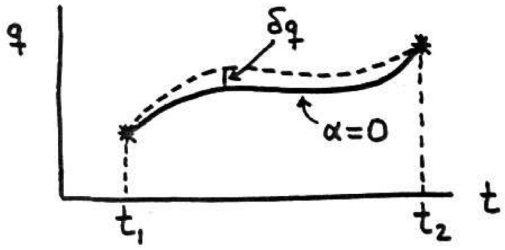

One way to parametrize different curves going from t_1 to t_2 is by a parameter α such that $\alpha = 0$ corresponds to the stationary value of I (see figure). The action is then written as

$$I(\alpha) = \int_{t_1}^{t_2} L[q(t,\alpha), \dot{q}(t,\alpha), t]dt. \tag{2.3}$$

A virtual variation for a fixed t is then

$$\delta q = \left(\frac{\partial q}{\partial \alpha}\right)_{\alpha=0} d\alpha, \ \delta \dot{q} = \left(\frac{\partial \dot{q}}{\partial \alpha}\right)_{\alpha=0} d\alpha. \tag{2.4}$$

The variation of I reads:

$$\delta I = \int_{t_1}^{t_2} [\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta \dot{q}]dt. \tag{2.5}$$

Since the variations are taking place at a fixed time, we may exchange the operations δ and d/dt so that $\delta \dot{q} = \frac{d}{dt}\delta q$. In this way, we obtain:

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$$\begin{aligned}\delta I &= \int_{t_1}^{t_2} \Big[\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\frac{d}{dt}\delta q\Big]dt, \\ &= \int_{t_1}^{t_2} \frac{\partial L}{\partial q}\delta q dt + \underbrace{\Big|_{t_1}^{t_2} \frac{\partial L}{\partial \dot{q}}\delta q}_{=0} - \int_{t_1}^{t_2} \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\delta q dt. \end{aligned} \tag{2.6}$$

The "surface term" (second term in the last line of the above equation) vanishes as there is no variation at the end points $t = t_1$ and $t = t_2$. Since the path taken by the system is determined by $\delta I = 0$, and since δq is arbitrary, it follows that the integrand itself must be zero:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0. \tag{2.7}$$

We have thus recovered Lagrange's equations. Generalized to multiple degrees of freedom, the same derivation above gives the same result with $q \to q_i$, $i = 1, 2, \ldots n$. We underline that the generalized coordinates have to be independent, in effect we are using holonomic constraints. The above procedure is valid for conservative systems [where $V = V(q_i)$] and non-conservative systems when $Q_i = -\frac{\partial U}{\partial q_i} + \frac{d}{dt}\frac{\partial U}{\partial \dot{q}_i}$ with $L = T - U$.

C. Variational calculus

The idea of finding the extremal value of an integral has practical use beyond the derivation of the Lagrange equations above. Let's say that we are interested in finding the extremal values of the integral

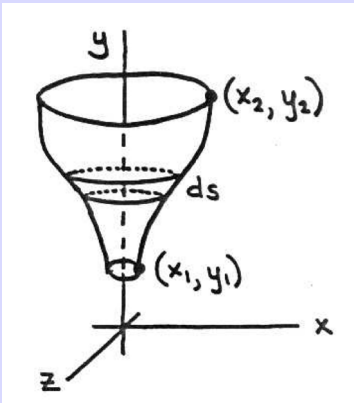
$$I = \int_{x_1}^{x_2} f(y, y', x)dx \tag{2.8}$$

where $f(y, y', x)$ is a function defined on the curve $y(x)$. Here, y' means dy/dx. The task is then to find the curve $y(x)$ which gives I its extremal value, in effect $\delta I = 0$. Now, we can simply reuse our result from the previous subsection. The function f which satisfies the following equations will give I an extremal value:

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} = 0. \tag{2.9}$$

In this context (variational calculus), these equations are known as the *Euler equations* or Euler-Lagrange equations. In practice, this would be a relevant problem to solve for instance if one wishes to minimize some quantity I with respect to a function f. To be concrete, I could be the amount of paint one has to use to paint a surface characterized by the function f. Let's use this as an example.

Example 6. Minimize surface area of an object. Consider a curve between two fixed points (x_1, y_1) and (x_2, y_2). Now revolve this curve around the y-axis to produce a surface (see figure). Our task is then to find the curve $y(x)$ which gives the minimal area of the surface of revolution.



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First, we need to find an expression for the area A of the surface. The area of the stripe ds is given as $2\pi x ds = 2\pi x\sqrt{dx^2+dy^2} = 2\pi x\sqrt{1+(y')^2}dx$. The total area is then given by integrating this from x_1 to x_2:

$$A = \int_{x_1}^{x_2} 2\pi x\sqrt{1+(y')^2}dx = 2\pi\int_{x_1}^{x_2} f(y,y',x)dx. \tag{2.10}$$

We defined $f(y,y',x) = x\sqrt{1+(y')^2}$. We can now use the Euler equations to find the curve f which makes A have an extremal value. Plugging f into equation (2.9), we get

$$\frac{d}{dx}\Big(\frac{xy'}{\sqrt{1+(y')^2}}\Big) = 0. \tag{2.11}$$

This equation may be solved for y as follows. The expression inside the paranthesis has to be a constant, let's call it a. Rewriting the expression in terms of y', we get

$$y' = \frac{dy}{dx} = \frac{a}{\sqrt{x^2-a^2}}. \tag{2.12}$$

Integrating with respect to x gives the solution

$$y = a\,\mathrm{acosh}(x/a) + b, \tag{2.13}$$

where b is the integration constant. Alternatively, we have $x = a\cosh[(y-b)/a]$. The boundary conditions $y(x_1) = y_1$ and $y(x_2) = y_2$ will then determine the coefficients a and b.

D. Hamilton's principle for non-holonomic systems

Up to now, we have mainly considered holonomic constraints. Recall that such constraints may be written mathematically as $f(\boldsymbol{r}_1,\dots\boldsymbol{r}_N,t) = 0$. Thus, with j holonomic constraints we were able to introduce $n = 3N-j$ generalized coordinates which were all independent. With n generalized coordinates and using our treatment above, Hamilton's principle becomes:

$$\int_{t_1}^{t_2} dt\sum_{k=1}^{n}\Big(\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial\dot{q}_k}\Big)\delta q_k = 0. \tag{2.14}$$

The argument which allowed us to set the integrand, rather than the entire integral, to zero was that all δq_k are independent. Thus, one arrives at Lagranges equations

$$\frac{d}{dt}\frac{\partial L}{\partial\dot{q}_k} - \frac{\partial L}{\partial q_k} = 0,\ k = 1,2,\dots n. \tag{2.15}$$

However, we are now considering non-holonomic systems and the main difference is that *not all δq_k are now independent*. To be concrete, let us assume that we have m constraints $f(q_i,\dot{q}_i,t) = 0$ (note the dependence on $\dot{q}_i$ which makes the constraint non-holonomic) of the rather general form:

$$a_{l,t}dt + \sum_{k=1}^{n} a_{l,k}dq_k = 0,\ l = 1,2,\dots m. \tag{2.16}$$

By dividing the entire equation on dt, we recast it into a form which depends on $\dot{q}_k$. The coefficients $a_{l,k}$ and $a_{l,t}$ are allowed to depend on the generalized coordinates q and time t, making the constraint above quite general. Any virtual displacements of the generalized coordinates δq_k have to be in accordance with the constraints

$$\sum_{k=1}^{n} a_{l,k}\delta q_k = 0. \tag{2.17}$$

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The reason δt does not enter the expression for the virtual displacement although it enters the constraint is that, as previously mentioned, virtual displacements take place at a fixed time t. In order to solve the problem, we will now make use of Lagranges method of undetermined multipliers. Recall that we have m equations (2.17) describing virtual displacements which are in accordance with the constraints of the system. Now multiply each of these equations with a coefficient $\lambda_l = \lambda_l(q,t)$.

$$\lambda_l \sum_{k=1}^{n} a_{l,k}\delta q_k = 0 \rightarrow \int_1^2 dt \sum_{l=1}^{m}\sum_{k=1}^{n} \lambda_l a_{l,k}\delta q_k = 0. \tag{2.18}$$

We can now combine this equation with Hamilton's principle derived previously, but with the important cavaet that we can *no longer use that the virtual displacements δq_k are independent of each other* due to the non-holonomic constraints. We thus have

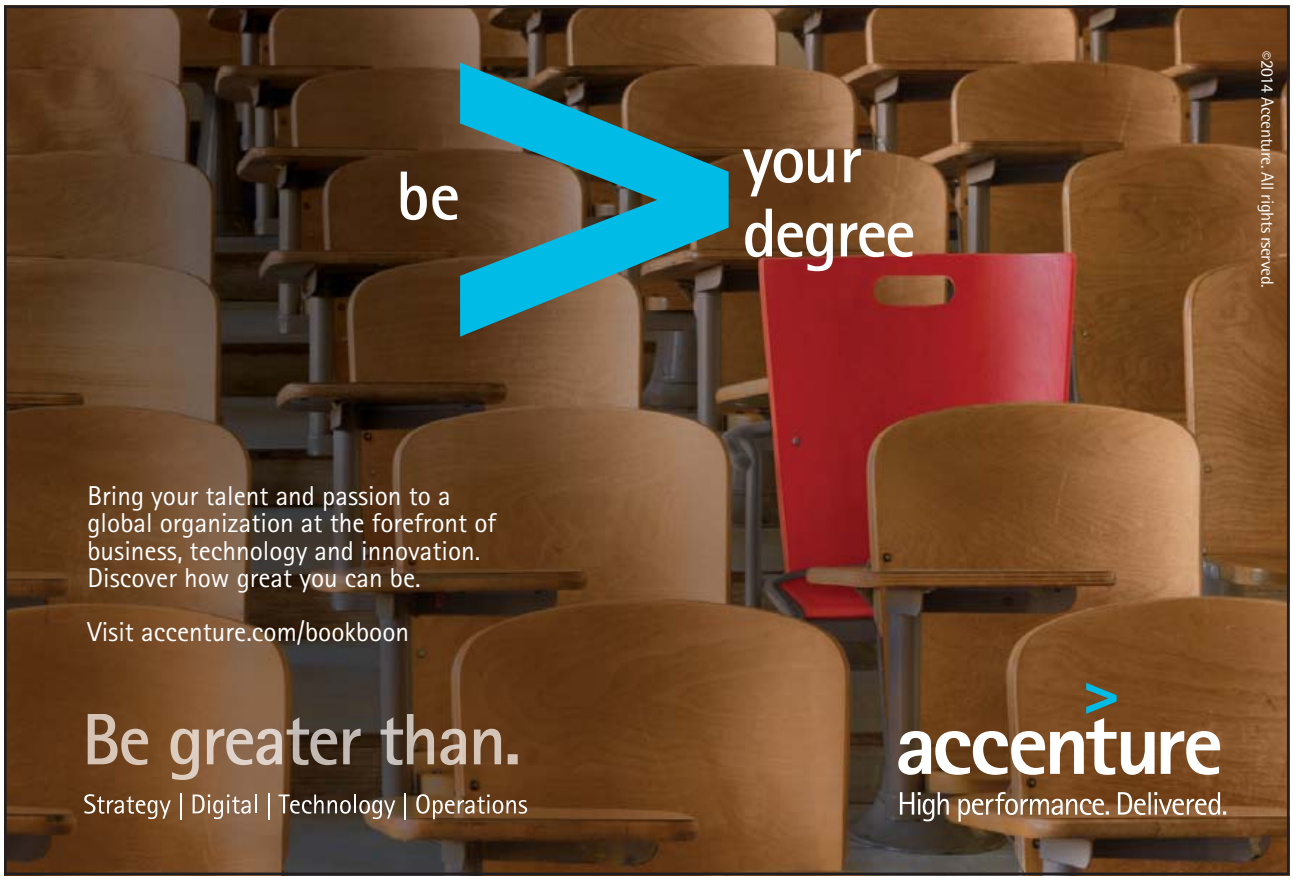
$$\int_1^2 dt \sum_{k=1}^{n} \Big(\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} + \sum_{l=1}^{m} \lambda_l a_{l,k}\Big)\delta q_k = 0. \tag{2.19}$$

We cannot set the integrand (the term inside the paranthesis to zero) immediately since the δq_k are not independent on each other. There are a lot of indices in play now, so let's clarify them a bit. We have in total n generalized coordinates. We also have $m < n$ non-holonomic constraints. This means that $n - m$ of the virtual displacements are independent on each other, whereas m of them do depend on each other via the relation equation (2.17).
Here is where we make use of the undetermined multipliers λ_l that we introduced. We have not specified them so far, but at this point it is useful to do so. In fact, let us *choose* them so that the equation

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} + \sum_{l=1}^{m} \lambda_l a_{l,k} = 0 \tag{2.20}$$

is satisfied for $k = n - m + 1, \ldots n$. In that case, equation (2.19) reduces to

$$\int_1^2 dt \sum_{k=1}^{n-m} \Big(\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} + \sum_{l=1}^{m} \lambda_l a_{l,k}\Big)\delta q_k = 0. \tag{2.21}$$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Now, we are left with only the virtual displacements δq_k which are independent on each other since the sum runs from 1 to $n-m$ and we *are* allowed to set the integrand to zero for all $k = 1, 2, \ldots n-m$. In total, we then have:

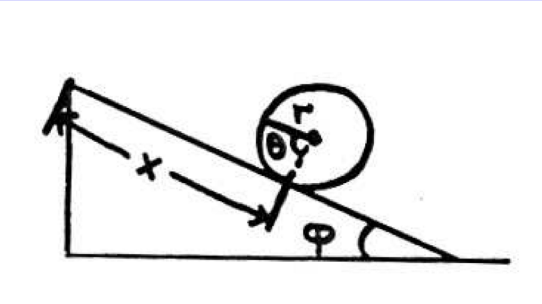
$$\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} + \sum_{l=1}^{m} \lambda_l a_{l,k} = 0, \ k = 1, 2, \ldots n. \tag{2.22}$$

These are the Lagrange equations which take into account the non-holonomic constraints. We have $n+m$ unknowns: n generalized coordinates $q_1, \ldots q_n$ and m Lagrange multipliers $\lambda_1, \ldots \lambda_m$. To find these unknowns, we then have n Lagrange equations and m constraints:

$$\sum_{k=1}^{n} a_{l,k}\dot{q}_k + a_{l,t} = 0, \ l = 1, 2, \ldots m. \tag{2.23}$$

We now show an example of how to use the Lagranger multiplier example in practice. Note that this technique can be used even when the constraints are holonomic, which makes it quite versatile.

Example 7. Ring rolling on an inclined plane.



Initially, it looks like we have two generalized coordinates x and θ. However, we also have a constraint present if the ring is supposed to always roll and never slide. The constraint is that the length $r \cdot d\theta$ of the edge segment that touches the ground has to be equal to the same distance dx along the inclined plane itself. By dividing $r \cdot d\theta = dx$ with dt on both sides, we see that this constraint has the same form as we considered in the previous subsection, namely

$$\sum_{k=1}^{2} a_k\dot{q}_k + a_t = a_x\dot{x} + a_\theta\dot{\theta} + a_t = 0, \tag{2.24}$$

if we set $a_x = 1$, $a_\theta = -r$, and $a_t = 0$. To proceed, we also need the Lagrange function $L = T - V$. According to the figure, we see that

$$\begin{aligned} T &= \frac{1}{2}M\dot{x}^2 + \frac{1}{2}Mr^2\dot{\theta}^2, \\ V &= Mg(l-x)\sin\phi. \end{aligned} \tag{2.25}$$

We defined l as the total length of the plane. We can now obtain Lagrange's equations for x and θ:

$$Mg\sin\phi - M\ddot{x} + \lambda = 0 \text{ and } Mr\ddot{\theta} = -\lambda. \tag{2.26}$$

Together with the constraint $\dot{x} = r\dot{\theta}$, we now have three equations and three unknowns (x, θ, λ). They are readily solved as follows:

$$\begin{aligned} \ddot{x} &= \frac{g\sin\phi}{2}, \\ \ddot{\theta} &= \frac{g\sin\phi}{2r}, \\ \lambda &= -\frac{Mg\sin\phi}{2}. \end{aligned} \tag{2.27}$$

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The acceleration when the ring slides is seen to be *half* of the acceleration it would have if it were to slide down the inclined plane without friction. In that case, we would have $\ddot{x} = g\sin\phi$ due to the gravitational acceleration. The reason for why the acceleration is now half as large is that the potential energy at the top of the plane has to be converted not only to kinetic energy for translational motion down the plane, but also for kinetic energy associated with rotational motion. The velocity of the ring at the bottom of the plane is found by integrating $\ddot{x} = \frac{1}{2}g\sin\phi$, yielding $v = \sqrt{gl\sin\phi}$.

The variational principle that we have discussed, whether in its differential or global form, has several advantages.

- It is most useful when one can find the Lagrange function expressed via independent coordinates (thus, for holonomic systems).
- This method involves only T and V which are physical quantities that are independent on the choice of coordinates. The whole formalism is thus invariant with respect to the choice of coordinates.
- The framework used above can be employed in several branches of physics. Consider for instance the following Lagrange function:

$$L = \frac{1}{2}\sum_j \mathcal{L}_j \dot{q}_j^2 + \frac{1}{2}\sum_{\substack{j,\,k \\ j\neq k}} M_{jk}\dot{q}_j\dot{q}_k - \sum_j \frac{q_j^2}{2C_j} + \sum_j E_j(t)q_j \tag{2.28}$$

  with the dissipation function $\mathcal{F} = \frac{1}{2}\sum_j R_j\dot{q}_j^2$. The resulting Lagrange equations read

$$\mathcal{L}_j\ddot{q}_j + \sum_{j\neq k} M_{jk}\ddot{q}_k + R_j\dot{q}_j + q_j/C_j = E_j(t) \tag{2.29}$$

  and can be used to describe systems as diverse as 1) a system of electrical circruits coupled via mutual inductances M_{jk} in which q above denotes the electric charges and 2) a system of masses and springs moving in a viscous medium where q now denotes the positions.

E. Conservation laws and symmetries

If the system we are considering have in total n degrees of freedom, there will be n second order differential equations that constitute the equations of motion. A complete solution would thus require 2 integrations per equation, leading to $2n$ integration constants that must be determined from the initial conditions (start-values for $q_1, \ldots q_n, \dot{q}_1, \ldots \dot{q}_n$.)

However, in many scenarios we are not necessarily interested in the exact solution for $q_j(t)$ for every $j = 1 \ldots n$. Instead, it can be more convenient to describe the nature of the system's motion in terms of *conservation laws and symmetries*.

To illustrate this, consider a system consisting of point masses moving in a potential V that only depends on position (i.e. a conservative potential). We then have:

$$\frac{\partial L}{\partial \dot{x}_i} = \frac{\partial T}{\partial \dot{x}_i} - \frac{\partial V}{\partial \dot{x}_i} = \frac{\partial T}{\partial \dot{x}_i} = m_i\dot{x}_i = p_{i,x}. \tag{2.30}$$

Note that summation over i is *not implied* in the second-last term in the above equation. With generalized coordinates q_i, we define the canonical momentum as

$$\boxed{p_i = \frac{\partial L}{\partial \dot{q}_i}}.$$

From the example above, we see that if the potential depends on velocity, the canonical momentum will be different from the mechanical momentum.

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Example 8. Particles in an electromagnetic field. As we have seen previously in this book, the appropriate Lagrangian for such a system reads

$$L = \frac{1}{2}\sum_i m_i \dot{\boldsymbol{r}}_i^2 - \sum_i q_i \phi(\boldsymbol{r}_i) + \sum_i q_i \boldsymbol{A}(\boldsymbol{r}_i)\cdot\dot{\boldsymbol{r}}_i. \tag{2.31}$$

From our definition of the canonical momentum, we find

$$p_{i,x} = \frac{\partial L}{\partial \dot{x}_i} = m_i\dot{x}_i + q_i A_x \neq m_i x_i. \tag{2.32}$$

Another very useful concept in the context of symmetries and conservation laws is cyclic coordinates:

A coordinate q_i is cyclic if L does not contain q_i. The belonging canonical momentum p_i is then constant.

To see this, we know that $\partial L/\partial q_i$ if q_i is cyclic which follows from its definnition. From the Lagrange equation, we then have

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{d}{dt}p_i = \dot{p}_i = 0, \tag{2.33}$$

so that p_i must be constant. Looking back on the above example with particles moving in an electromagnetic field, we see that if the scalar potential ϕ and vector potential $\boldsymbol{A}$ are both independent on x, then L is independent on x and x is a cyclic coordinate. The canonical momentum $p_x = m\dot{x} + qA_x$ is then constant, while the *mechanical momentum* $m\dot{x}$ is not conserved.

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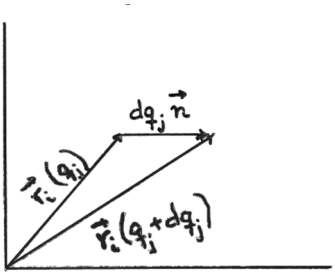
What we have seen so far is that there appears to be a relation between a symmetry (meaning an operation which leaves L invariant) and a conservation law (a quantity which remains constant). In other words, when the system has a symmetry, something is often conserved. This is not a coincidental relation, but actually a very profound result in theoretical physics known as **Noether's theorem**:

If a system has a *continuous* symmetry, there exists a quantity whose value is time-independent.

It is important to emphasize here that this holds for continuous symmetries, and not necessarily discrete symmetries (such as reflection $\boldsymbol{r} \to -\boldsymbol{r}$.)

We will now examine more closely which conservation laws that arise in the context of translational and rotational symmetries. Finally, we will also discuss the symmetry which leads to the pivotal energy conservation law (can you already now guess which symmetry this is?)

Let us start off with *translational symmetry*. Consider a generalized coordinate q_j which is defined so that dq_j means translation of the entire system in a direction $\boldsymbol{n}$.



From the figure, it is clear that for all i we have:

$$\frac{\partial \boldsymbol{r}_i}{\partial q_j} = \lim_{dq_j \to 0} \frac{\boldsymbol{r}_i(q_j + dq_j) - \boldsymbol{r}_i(q_j)}{dq_j} = \frac{dq_j \boldsymbol{n}}{dq_j} = \boldsymbol{n}. \tag{2.34}$$

Assume that we have a conservative system, $V = V(q)$. The Lagrange-equation

$$\frac{d}{dt}\frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} = Q_j \tag{2.35}$$

holds in general for a holonomic system, as discussed earlier. Velocities, and thus T, are not affected by moving the origo such that $\partial T/\partial q_j = 0$. It follows, by using the definition of the generalized force Q_j:

$$\dot{p}_j = Q_j = \sum_i \boldsymbol{F}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} = \boldsymbol{F} \cdot \boldsymbol{n}. \tag{2.36}$$

In effect, Q_j is the component of the total force $\boldsymbol{F}$ along the direction $\boldsymbol{n}$. The canonical momentum may be computed as follows:

$$p_j = \frac{\partial T}{\partial \dot{q}_j} = \sum_i m_i \dot{\boldsymbol{r}}_i \cdot \frac{\partial \dot{\boldsymbol{r}}_i}{\partial \dot{q}_j} = \sum_i m_i \dot{\boldsymbol{r}}_i \cdot \frac{\partial \boldsymbol{r}_i}{\partial q_j} = \sum_i m_i \boldsymbol{v}_i \cdot \boldsymbol{n} = \boldsymbol{P} \cdot \boldsymbol{n}. \tag{2.37}$$

Thus, p_j is the component of the total linear momentum $\boldsymbol{P}$ along $\boldsymbol{n}$. If q_j is cyclic, then $\partial L/\partial q_j = 0$ and p_j is conserved.

Next, we consider *rotational symmetry*. Consider a generalized coordinate q_j which is such that dq_j means a rotation of the entire system around an axis $\boldsymbol{n}$. Using the same arguments as above, we again find that $p_j = Q_j$ with $Q_j = \sum_i \boldsymbol{F}_i \cdot \partial \boldsymbol{r}_i / \partial q_j$.

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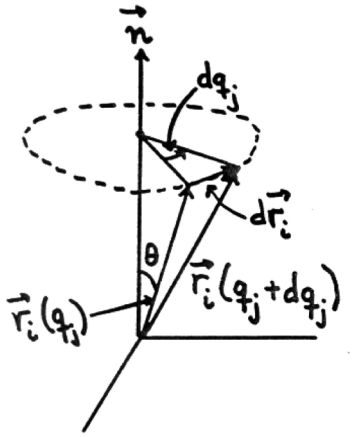

From the figure, we see that

$$|d\boldsymbol{r}_i| = r_i \sin\theta dq_j \rightarrow \left|\frac{\partial \boldsymbol{r}_i}{\partial q_j}\right| = r_i \sin\theta \tag{2.38}$$

where the vector on the right side of the equation has a direction perpendicular to both $\boldsymbol{r}_i$ and $\boldsymbol{n}$. Thus, we have

$$\frac{\partial \boldsymbol{r}_i}{\partial q_j} = \boldsymbol{n} \times \boldsymbol{r}_i. \tag{2.39}$$

Using these relations, we may compute the generalized force

$$Q_j = \sum_i \boldsymbol{F}_i \cdot (\boldsymbol{n} \times \boldsymbol{r}_i) = \sum_i \boldsymbol{n} \cdot (\boldsymbol{r}_i \times \boldsymbol{F}_i) = \boldsymbol{n} \cdot \boldsymbol{\tau}. \tag{2.40}$$

Here, $\boldsymbol{\tau}$ is the total torque acting on the system. In the same way, we identify

$$p_j = \sum_i m_i \boldsymbol{v}_i \cdot (\boldsymbol{n} \times \boldsymbol{r}_i) = \boldsymbol{n} \cdot \boldsymbol{L}. \tag{2.41}$$

Summarizing so far, Q_j is the component of the angular torque along $\boldsymbol{n}$ and p_j is the component of the angular momentum along $\boldsymbol{n}$. If q_j is cyclic, it follows that $Q_j = 0$ so that p_j is conserved. In other words, when the system is invariant under rotation around an axis, the component of the angular momentum along that axis is conserved.

Finally, we consider conservation of energy. This is a conservation law that is often taken for granted, but there is actually a specific requirement that must be fulfilled in order for energy to be conserved. Assume that we have a Lagrange function $L = L(q_i, \dot{q}_i, t)$ with a potential $V = V(q_i)$. Now the total derivative is:

$$\begin{aligned} dL/dt &= \sum_i \frac{\partial L}{\partial q_i}\frac{dq_i}{dt} + \sum_i \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt} + \frac{\partial L}{\partial t} \\ &= \sum_i \frac{d}{dt}[\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i] + \frac{\partial L}{\partial t}. \end{aligned} \tag{2.42}$$

Moving the left-hand side over to the right side, we get the equation

$$\frac{dH}{dt} + \frac{\partial L}{\partial t} = 0, \tag{2.43}$$

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where we defined the energy function (or the *Hamilton* function)

$$H(q,\dot{q},t) = \sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i - L. \tag{2.44}$$

It follows that if L has no explicit time-dependence, i.e. $\partial L/\partial t = 0$, then $dH/dt = 0$. To proceed, we note that the mathematical property that for a homogeneous function f of the n-th degree, Euler's theorem dictates:

$$\sum_i x_i \frac{\partial f}{\partial x_i} = nf \tag{2.45}$$

It so happens that the kinetic energy T is a homogeneous function of the 2nd degree, meaning that

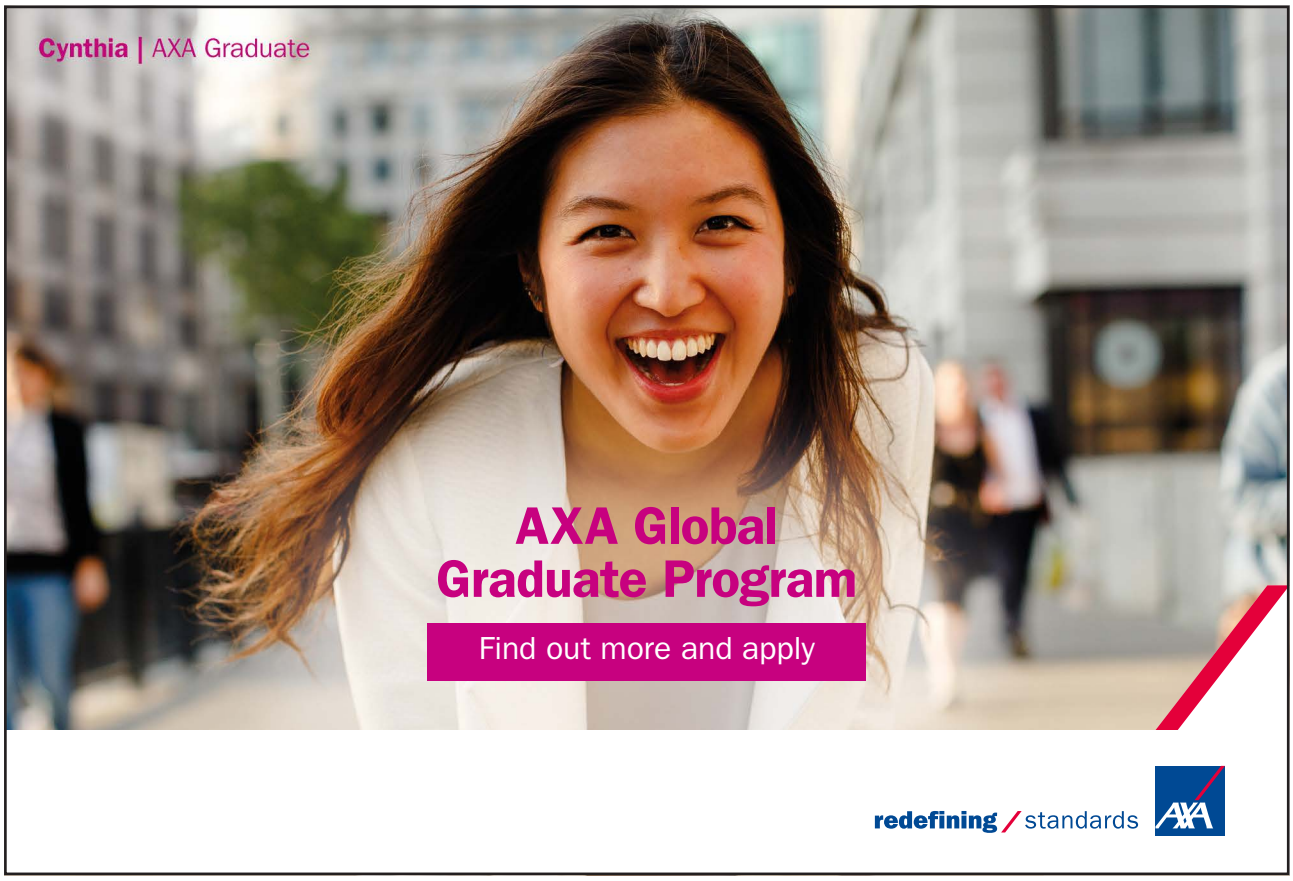
$$\sum_i \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = \sum_i \dot{q}_i m_i \dot{q}_i = 2T. \tag{2.46}$$

To get this result, we used that $\partial L/\partial \dot{q}_i = \partial T/\partial \dot{q}_i$ since the system is conservative. Using the above result, we then have

$$H = 2T - L = 2T - (T - V) = T + V = \text{total energy}. \tag{2.47}$$

In other words:

If the Lagrange function has no explicit time-dependence, $\partial L/\partial t = 0$ and the total energy of the system is conserved.



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III. HAMILTON'S EQUATIONS

Youtube-videos. 11-12 in this playlist.

Learning goals. After reading this chapter, the student should:

- Understand how Hamilton's and Lagrange's equations are related and obtained from one another.
- Know how to construct and solve Hamilton's equations for simple model systems.

A. Legendre transformations

Upon introducing Hamilton's equations in this chapter, we emphasize right away that these are equivalent to Lagrange's equations - there is no new physics involved, just a new method or technique. In terms of directly solving problems in mechanics, Hamilton's equations are not better or worse than the Lagrange formalism. However, the Hamiltonian framework is more suitable in other areas of physics, including quantum mechanics and statistical mechanics. In what follows, we shall consider holonomic systems with monogenic forces. According to our previous definition of these concepts, we then have $V = V(q)$ or $U = U(q, \dot{q})$ (the latter as in the case of an electromagnetic field). Even with these restrictions, the following analysis remains valid for a vast number of physical situations.

Let us first briefly recap. The Lagrange formulation may be stated as follows:

With n degrees of freedom, we have $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$, $i = 1, 2, \ldots n$. We thus have n second order differential equations: a complete solution requires $2n$ initial conditions, such as the values of q_i and $\dot{q}_i$ at one time t_1 or alternatively the values of q_i at two times t_1 and t_2. The state of the system is specified by a point in the n-dimensional configuratiotn space with axes q_i.

Instead, the Hamilton formulation may be summarized as follows:

With n degrees of freedom, we have $2n$ first order differential equations. We thus still need $2n$ initial conditions. The state of the system is specified by a point in the $2n$-dimensional *phase space* with axes q_i and p_i where

$$p_i = \frac{\partial L(q_j, \dot{q}_j, t)}{\partial \dot{q}_i}, \; i = 1, 2, \ldots n \tag{3.1}$$

The quantities q and p are known as canonical variables.

From a mathematical perspective, the transition from Lagrange to Hamilton formulation requires that we change the variables in our functions from $(q, \dot{q}, t)$ to (q, p, t) where $p = \partial L/\partial \dot{q}$. There actually exists a specific recipe to accomplish such a change in variables known as the Legrendre transformation which we now review.

Assume that we have a function $f(x, y)$ such that

$$df = u \cdot dx + v \cdot dy \tag{3.2}$$

with $u = \partial f/\partial x$ and $v = \partial f/\partial y$. We now wish to change basis from (x, y) to (u, y) so that differentials are expressed via du and dy. Let us define

$$g = f - ux \tag{3.3}$$

It is no coincidence that the new function is defined as the old one minus the *product between the variables that we want to interchange*, namely u and x in this particular case. In this way, we see that

$$dg = df - u \cdot dx - x \cdot du = v \cdot dy - x \cdot du. \tag{3.4}$$

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This is the desired form. Since we also have generically $dg = (\partial g/\partial u)du + (\partial g/\partial y)dy$, it follows that

$$x = -\partial g/\partial u,\ v = \partial g/\partial y. \tag{3.5}$$

The Legendre transformation is commonly used in thermodynamics. Let's have a look at an example.

Example 9. Use of Legendre transformation in thermodynamics. Enthalpy H (not to be confused with the Hamiltonian) is a function of entropy S and pressure p in the following way:

$$\partial H/\partial S = T,\ \partial H/\partial p = V. \tag{3.6}$$

The enthalpy $H = H(S, p)$ is useful in particular for isentropic and isobaric processes since it remains constant. However, if one instead is interested in describing isothermic and isobaric processes it is more convenient to use a function depending on T and p. We now know how to accomplish this - via a Legendre transformation. The new function is supposed to be the old one minus the product of the two variables we wish to exchange, S and T in this case. We thus define

$$G = H - TS \tag{3.7}$$

so that

$$dG = dH - T \cdot dS - S \cdot dT = T \cdot dS + V \cdot dp - T \cdot dS - S \cdot dT = V \cdot dp - S \cdot dT. \tag{3.8}$$

Here, G is the Gibbs free energy.

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B. Going from Lagrangian to Hamiltonian formalism

The natural Legendre transformation for going from the Lagrange to Hamilton formalism is then taking the difference between the product of the coordinates to be exchanged and the old function:

$$H = H(q, p, t) = p\dot{q} - L. \tag{3.9}$$

There are two ways to express the differential dH:

$$dH = \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial t} dt \tag{3.10}$$

while from Eq. (3.9) we get

$$dH = \dot{q}_i \cdot dp_i + p_i \cdot d\dot{q}_i - \frac{\partial L}{\partial q_i} dq_i - \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i - \frac{\partial L}{\partial t} dt. \tag{3.11}$$

Since $p_i = \partial L / \partial \dot{q}_i$, it follows that:

$$dH = \dot{q}_i \cdot dp_i - \dot{p}_i \cdot dq_i - \frac{\partial L}{\partial t} dt. \tag{3.12}$$

It is useful to note here that by dividing the above equation on dt, it follows that $dH/dt = -\partial L/\partial t$. By direct comparison, with Eq. (3.10), we can now immediately write down Hamilton's canonical equations:

$$\boxed{\dot{q}_i = \frac{\partial H}{\partial p_i},\ \dot{p}_i = -\frac{\partial H}{\partial q_i},\ \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}.}$$

We may then summarize the procedure used in the Hamilton formalism to solve a given problem:

- Construct $L = L(q, \dot{q}, t)$.
- Define the canonical momenta $p_i = \partial L / \partial \dot{q}_i$.
- Construct the Hamilton function $H = p_i \dot{q}_i - L$.
- Use $p_i = \partial L / \partial \dot{q}_i$ to express $\dot{q}_i$ as a function of (q, p, t).
- Eliminate $\dot{q}_i$ from H such that $H = H(q, p, t)$.
- You can now use H to solve the canonical equations of motion.

Let's have a look at a practical example of this.

Example 10. Hamilton formalism for particle in EM field. We know from previous considerations in this book that for this scenario we have $L = T - U$ with $U = q\phi - q\boldsymbol{A} \cdot \boldsymbol{v}$. The potentials ϕ and $\boldsymbol{A}$ may depend on $\boldsymbol{r}$ and t. The Lagrange equations are satisfied with this U:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0. \tag{3.13}$$

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Using Cartesian coordinates and the sum convention, we may write

$$L = \frac{1}{2}m\dot{x}_i\dot{x}_i + qA_i\dot{x}_i - q\phi. \tag{3.14}$$

The canonical momentum is then

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + qA_i. \tag{3.15}$$

From this, we obtain the Hamilton function

$$H = p_i\dot{x}_i - L = (m\dot{x}_i + qA_i)\dot{x}_i - \frac{1}{2}m\dot{x}_i\dot{x}_i - qA_i\dot{x}_i + q\phi = \frac{1}{2}m\dot{x}_i\dot{x}_i + q\phi. \tag{3.16}$$

This is simply mechanical (kinetic) energy pluss potential energy. We now get rid off $\dot{x}_i$ via

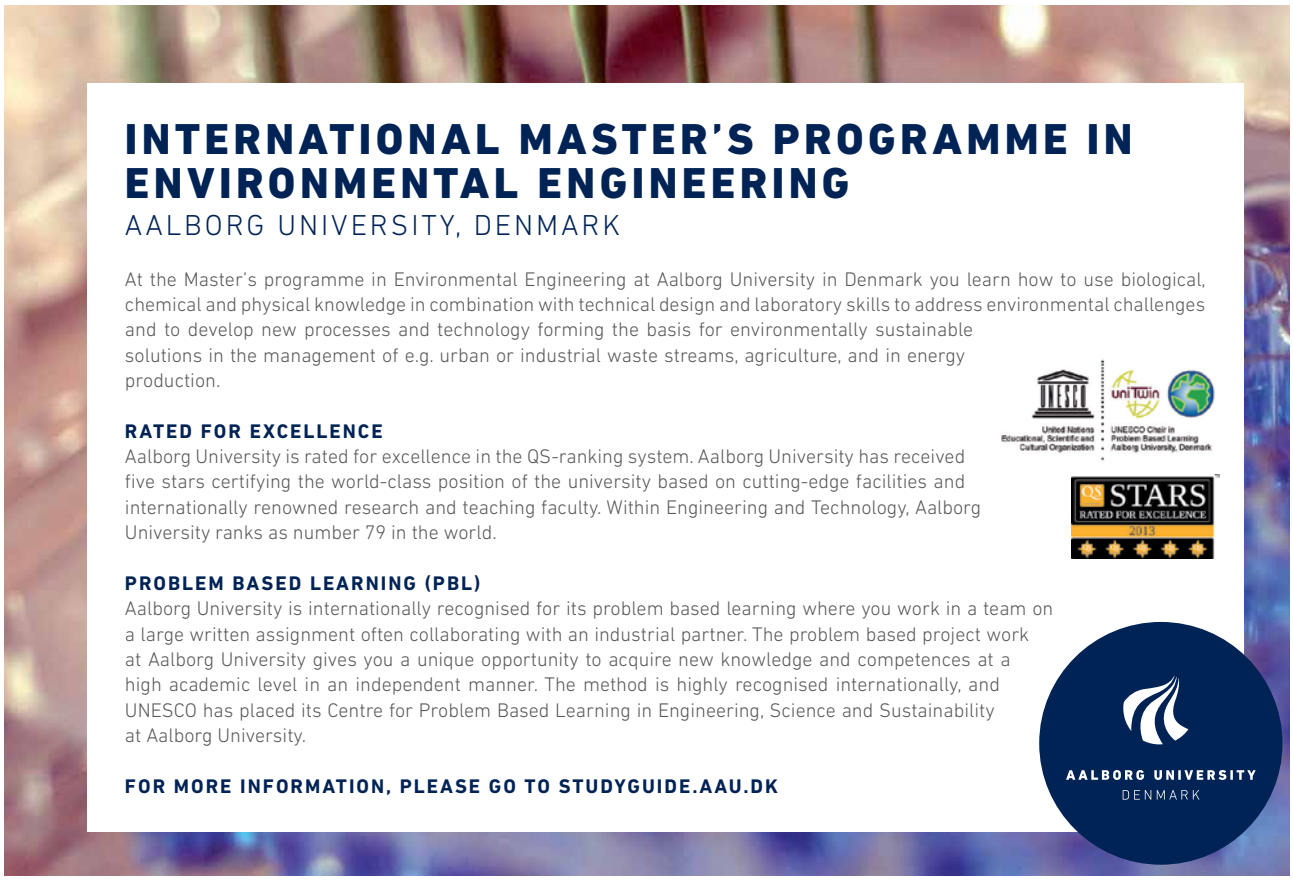
$$\dot{x}_i = \frac{1}{m}(p_i - qA_i) \tag{3.17}$$

and upon insertion of this into H we end up with

$$H = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A})^2 + q\phi \tag{3.18}$$

where the dependence on x_i and t is in $\boldsymbol{A}$ and ϕ. Thus, if $\boldsymbol{A}$ and ϕ are independent on t we have $\partial L/\partial t = 0$ and thus the Hamilton function is conserved:

$$dH/dt = \partial H/\partial t = -\partial L/\partial t = 0. \tag{3.19}$$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IV. THE TWO-BODY PROBLEM: CENTRAL FORCES

Youtube-videos. 13-20 in this playlist.

Learning goals. After reading this chapter, the student should:

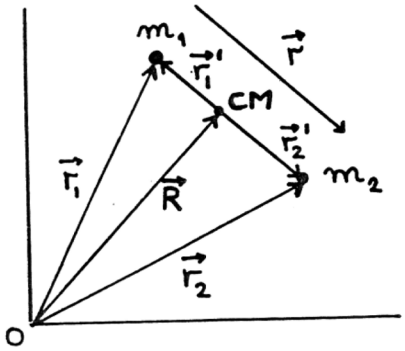
- Be able to explain and derive how a two-body problem with central force interactions can be reduced to an effective one-body problem.
- Understand how different particle trajectories arise depending on the energy E of the particle and classify these trajectories accordingly
- Have detailed knowledge on how to treat a particle moving in a Kepler potential
- Understand the concept of a differential scattering cross section and be able to compute it for simple potential profiles $V(r)$

A. Reduction to equivalent one-body problem

A powerful result in treating a two-body system where the forces are central (i.e. acting only along the line connecting the two bodies) is that the system may be reduced to an effective one-body problem. We will now derive exactly how this equivalency is obtained.

With two classical bodies, there are in general 6 degrees of freedom (3 d.o.f. for each body associated with movement in the three spatial dimensions). This means we need 6 generalized coordinates to describe the total system. We may choose for instance the CoM coordinate $\boldsymbol{R}$ and the relative coordinate $\boldsymbol{r}$:

$$\boldsymbol{R} = \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{m_1 + m_2},\ \boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1. \tag{4.1}$$



If the force resulting from the interaction between the particle is central, we have a potential

$$V = V(r),\ r = |\boldsymbol{r}|. \tag{4.2}$$

The Lagrange function is then

$$L = T(\dot{\boldsymbol{R}}, \dot{\boldsymbol{r}}) - V(r). \tag{4.3}$$

Let us consider the kinetic energy in more detail. We have

$$T = \frac{1}{2}m_1\dot{\boldsymbol{r}}_1^2 + \frac{1}{2}m_2\dot{\boldsymbol{r}}_2^2 \tag{4.4}$$

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which after straightforward algebraic manipulation may be re-expressed in terms of $\boldsymbol{R}$ and $\boldsymbol{r}$ as follows

$$T = \frac{1}{2}(m_1 + m_2)\dot{\boldsymbol{R}}^2 + \frac{1}{2}\frac{m_1 m_2}{m_1 + m_2}\dot{\boldsymbol{r}}^2. \tag{4.5}$$

At this point, it is convenient to introduce the reduced mass $\mu \equiv m_1 m_2/(m_1 + m_2)$ and the total mass $M = m_1 + m_2$. We then have

$$L = \frac{1}{2}M\dot{\boldsymbol{R}}^2 + \frac{1}{2}\mu\dot{\boldsymbol{r}}^2 - V(r) \tag{4.6}$$

The crucial observation at this point is now that $\boldsymbol{R}$ is a cyclic coordinate: L is independent on $\boldsymbol{R}$. It follows that the belonging canonical momentum $p_{\boldsymbol{R}}$ must be a constant:

$$p_{\boldsymbol{R}} = \frac{\partial L}{\partial \dot{\boldsymbol{R}}} = M\dot{\boldsymbol{R}} = \text{constant}. \tag{4.7}$$

Thus, $\dot{\boldsymbol{R}}$ is a constant and we may simply drop the term $M\dot{\boldsymbol{R}}^2$ since adding or subtracting a constant to a Lagrange function has no physical consequence: it simply redefines the zero-energy level of the potential energy. With this simplification, we have now in fact reduced the initial two body problem to an equivalent one body problem since L now only depends on $\boldsymbol{r}$ and $\dot{\boldsymbol{r}}$:

$$L = T - V = \frac{1}{2}\mu\dot{\boldsymbol{r}}^2 - V(r) \tag{4.8}$$

In other words, the physics of the system corresponds to a particle with mass μ moving with a velocity $\dot{\boldsymbol{r}}$ (where $\boldsymbol{r}$ is the relative coordinate between the original two bodies) in a potential $V(r)$.

B. Equations of motion

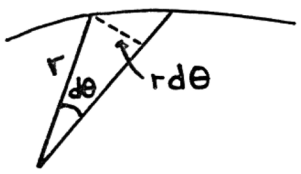
Since we will consider the one body Lagrange function, let us simply rename $\mu \to m$. We are then looking at a mass m in a central forcefield. The system is rotationally symmetric as the force only depends on the distance r and it follows that angular momentum must be conserved:

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} \tag{4.9}$$

We remind the reader that whenever a continuous symmetry is present, meaning that L is invariant under some continuous operation such as an arbitrary rotation, there must be a belonging conservation law. Both the magnitude and size of $\boldsymbol{L}$ is conserved, which can only be fulfilled if $\boldsymbol{r}$ always lies in a plane perpendicular to $\boldsymbol{L}$. Central motion thus always occurs in a plane. For this reason, we only need polar-coordinates r and θ to fully describe the problem. We then have

$$L = T - V = \frac{1}{2}m(\dot{\boldsymbol{r}}^2 + r^2\dot{\theta}^2) - V(r) = L(\boldsymbol{r}, \dot{\boldsymbol{r}}, \dot{\theta}). \tag{4.10}$$

Since θ is cyclic, $p_\theta = mr^2\dot{\theta}$ must be conserved. In fact, $mr^2\dot{\theta} \equiv l$ is the magnitude of the angular momentum. One of the equations of motion is then $\dot{p}_\theta = \frac{d}{dt}(mr^2\dot{\theta}) = 0$. We can now prove Kepler's 2nd law, which demonstrates that for the present mass moving in a central forcefield, the radius of the trajectory of the mass sweeps over equally large areas for any equally large time intervals.



It follows from the figure that $dA = \frac{1}{2}r \cdot r \cdot d\theta$. In effect, $\dot{A} = \frac{1}{2}r^2\dot{\theta} = p_\theta/(2m)$ which is a constant. The second equation of motion comes from Lagrange's equation for the coordinate r and reads:

$$\frac{d}{dt}(m\dot{r}) - mr\dot{\theta}^2 + \frac{\partial V}{\partial r} = 0. \tag{4.11}$$

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The force in $\boldsymbol{r}$-direction is $f(r) = -\partial V/\partial r$. We then have

$$m\ddot{r} - mr\dot{\theta}^2 = f(r). \tag{4.12}$$

One can now eliminate $\dot{\theta}$ via $mr^2\dot{\theta} = l$, and thus

$$m\ddot{r} - \frac{l^2}{mr^3} = f(r). \tag{4.13}$$

This is a 2nd order differential equation in one single variable: r. For a conservative system, we know that not only l but also the energy E is a conserved quantity:

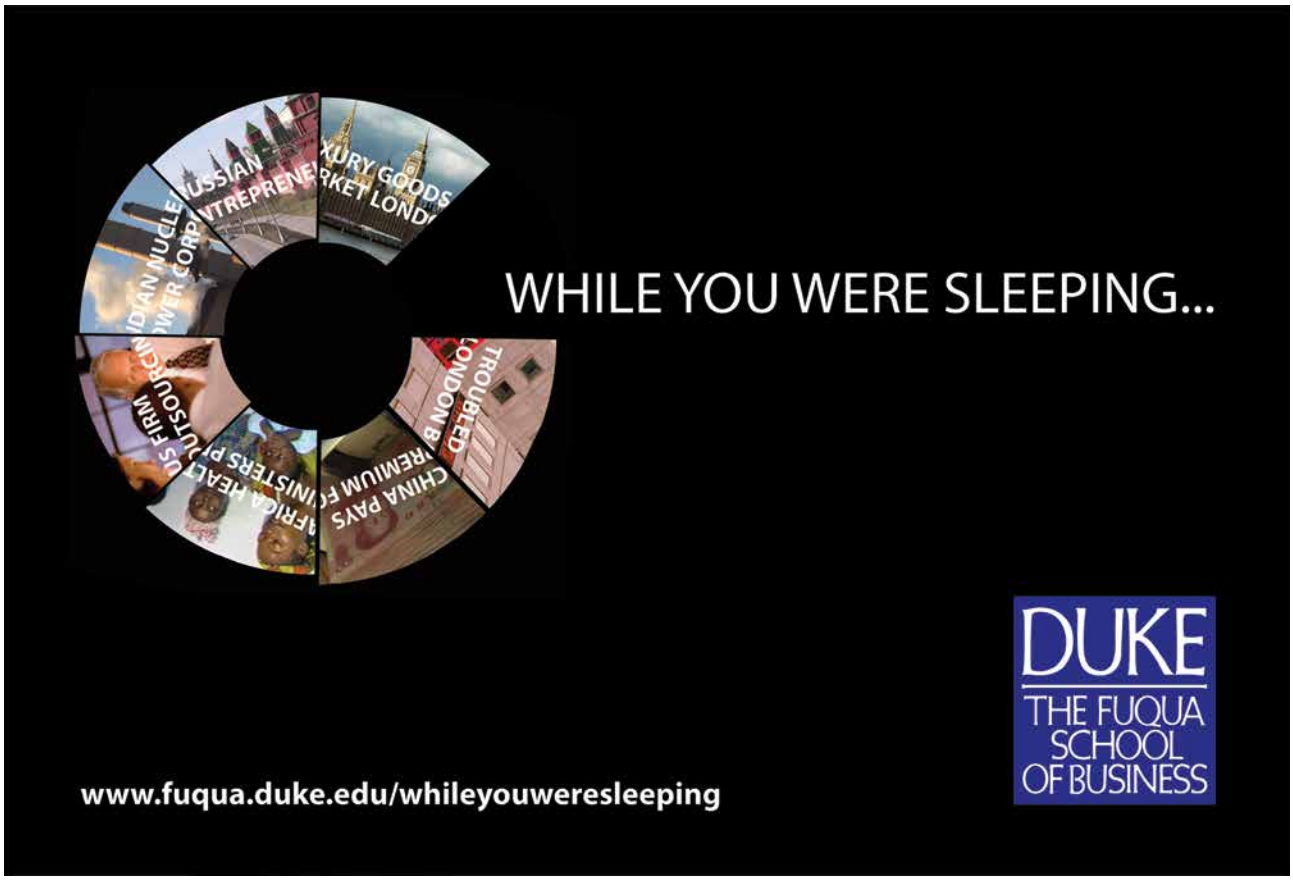
$$E = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + V(r). \tag{4.14}$$

C. Equivalent one-dimensional problem

So far, we have not specified the exact form of $V(r)$. For an arbitrary $V(r)$, the differential equation cannot be solved in general. However, it is possible to gain physical insight in the behavior of the particle m even in this case by utilizing an analogy for one-dimension. To do so, note that Eq. (4.13) may be rewritten as

$$m\ddot{r} = f'(r) = f(r) + l^2/mr^3. \tag{4.15}$$

This has the same form as Newton's 2nd law for a one-dimensional problem where a mass m is affected by a force $f'(r)$. The extra term in $f'(r)$ besides the external potential $f(r)$ is the *centrifugal force*. The corresponding effective potential $V'(r)$ may be written $V'(r) = V(r) + l^2/2mr^2$. In order to see which consequence this extra term has, we may consider a specific example with $V(r) = -k/r$. It is instructive to plot the effective potential $V'(r)$ as shown below.



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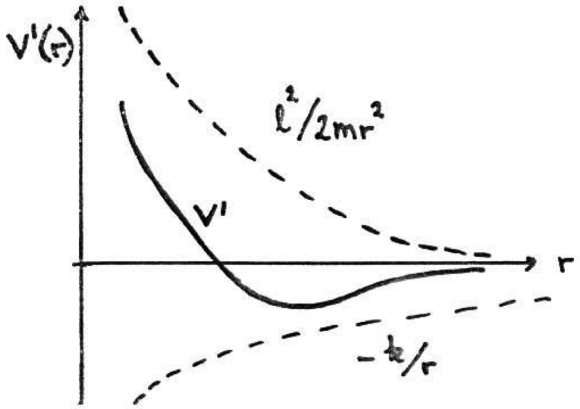
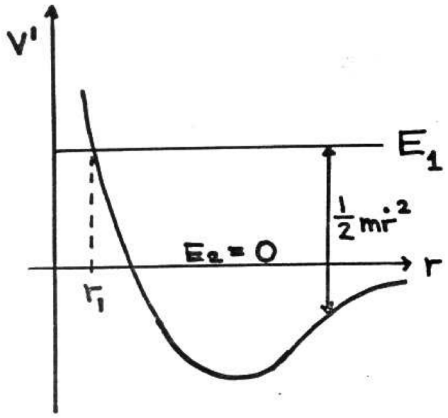
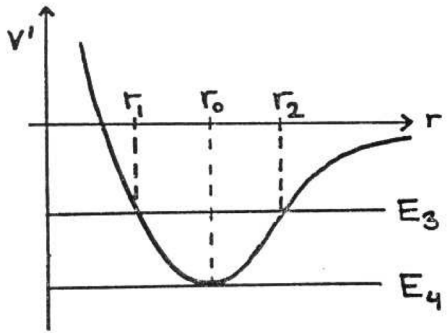


We see that $\lim_{r\to 0} V'(r) = +\infty$ and $\lim_{r\to\infty} V'(r) = -0$. The trajectory of a particle moving in this potential will depend on its energy E. We may distinguish between four particular scenarios.





- $E > 0$: the particle cannot access radii smaller than r_1 if its energy is $E = E_1$, while there is no upward bound on r. It thus has a turning point at $r = r_1$.
- $E = 0$: qualitatively the same type of motion as for $E > 0$.
- $E < 0$: The motion is now completely bounded: the particle may only have positions within the radii r_1 and r_2, i.e. $r_1 < r < r_2$.
- $E = E_{\text{min}}$: The particle can only occupy one particular radius $r = r_0$, which means its trajectory must be a circle since $\dot{r} = 0$. This scenario takes place when the force from the external potential matches exactly the centrifugal force.

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D. The virial theorem

We here briefly discuss a useful result known as the virial theorem, which for instance finds its use when discussing periodic motion (such as planetary motion). It is a general theorem valid for many different physical systems due to its statistical nature. Assume that the system under consideration has masses in positions $\boldsymbol{r}_i$ and that the masses are affected by forces $\boldsymbol{F}_i$, which includes any forces resulting from constraints. We then have $\dot{\boldsymbol{p}}_i = \boldsymbol{F}_i$ and by defining the quantity

$$G = \sum_i \boldsymbol{p}_i \cdot \boldsymbol{r}_i \tag{4.16}$$

it follows that

$$\frac{dG}{dt} = \sum_i \dot{\boldsymbol{r}}_i \cdot \boldsymbol{p}_i + \sum_i \dot{\boldsymbol{p}}_i \cdot \boldsymbol{r}_i. \tag{4.17}$$

We may rewrite this as

$$\frac{dG}{dt} = 2T + \sum_i \boldsymbol{F}_i \cdot \boldsymbol{r}_i. \tag{4.18}$$

Now, let us average this equation over a time interval τ, leading to ($\overline{\cdots}$ denoting time-averaging):

$$\frac{1}{\tau}[G(\tau) - G(0)] = 2\overline{T} + \overline{\sum_i \boldsymbol{F}_i \cdot \boldsymbol{r}_i}. \tag{4.19}$$

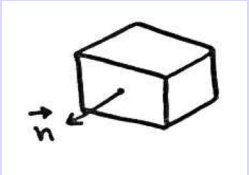
If the motion is periodic and τ is its period, we see that the left hand side is 0. If the motion is not periodic while $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ are always finite (which is reasonable), then $\lim_{\tau\to\infty}$ of the left hand side also gives zero. Thus, in both cases we obtain

$$\bar{T} = -\frac{1}{2}\overline{\sum_i \boldsymbol{F}_i \cdot \boldsymbol{r}_i}. \tag{4.20}$$

This is the virial theorem which thus provides a relation between the average kinetic energy of the system and the forces acting on its constituents. Let's look at some examples.

Example 11. Ideal gas. Consider an ideal gas with volume V and N atoms. According to the equipartition principle from statistical mechanics, we know that $\overline{T} = 3NkT/2$. This is obtained by each particle providing an average kinetic energy of $kT/2$ for each degree of freedom in its motion. Let $\boldsymbol{F}_i$ be the force exerted on the atoms by the wall, so that $d\boldsymbol{F}_i = -p\boldsymbol{n}dA$ where p is the pressure of the gas. Since we assume an ideal gas, interactions between the atoms themselves are neglected. We then obtain:

$$\frac{1}{2}\overline{\sum_i \boldsymbol{F}_i \cdot \boldsymbol{r}_i} = -\frac{1}{2}p\int \boldsymbol{n}\cdot\boldsymbol{r}dA = -\frac{1}{2}p\int(\nabla\cdot\boldsymbol{r})dV = -\frac{3}{2}pV. \tag{4.21}$$



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Example 12. Particle in a central force field. For conservative forces, we have $\boldsymbol{F}_i = -\nabla_i V$. Thus, $\overline{T} = \frac{1}{2}\overline{\sum_i \nabla_i V \cdot \boldsymbol{r}_i}$. Assume we have one single particle moving in a central field:

$$\overline{T} = \frac{1}{2}\overline{\frac{\partial V}{\partial r} r} \tag{4.22}$$

If the potential is given generally by a power-law dependence on the radius, i.e. $V = ar^{n+1}$ (so that the force itself goes like r^n), we obtain $\overline{T} = \frac{n+1}{2}\overline{V}$. For the special case of a harmonic oscillator $(n = 1)$, we get $\overline{T} = \overline{V}$. In effect, the average kinetic energy is equal to the average potential energy.

E. The Kepler problem

We will now consider in great detail a potential of particular importance, relevant *e.g.* for planetary motion in our solar system. We take the force to be $F(r) = -k/r^2$, so that the potential is $V(r) = -k/r$. This is the so called Kepler potential. The task is to determine the trajectory that a particle moving in this potential will take, i.e. to find $r = r(\theta)$.

We have that, generally, $\dot{r} = \sqrt{(2/m)(E - V - l^2/2mr^2)}$. By using $\dot{r} = dr/dt$ and combining this equation with $\dot{\theta} = l/mr^2$ (where $\dot{\theta} = d\theta/dt$), we obtain

$$d\theta = \frac{l dr}{mr^2\sqrt{\frac{2}{m}(E - V - l^2/2mr^2)}}. \tag{4.23}$$

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This integral can be solved:

$$\theta - \theta_0 = \int_{r_0}^{r} \frac{dr}{r^2\sqrt{\frac{2mE}{l^2} - \frac{2mV}{l^2} - \frac{1}{r^2}}}. \tag{4.24}$$

So far, the treatment is valid for a general potential $V(r)$. Now, we insert our Kepler potential $V(r) = -k/r$ and use the substitution $u = 1/r$ (so that $du = -dr/r^2$):

$$\theta - \theta_0 = -\int \frac{du}{\sqrt{\frac{2mE}{l^2} + \frac{2mku}{l^2} - u^2}}. \tag{4.25}$$

The integration constant θ_0 is determined by the initial conditions. For now, let us set $\theta_0 = 0$. We will see from the final solution that this choice means that we are measuring the polar angle θ relative the *perihelion* of the trajectory. This is defined as the point where the particle is closest to the center of the potential ($r = 0$). The above integral over u has a solution analytically, by using the following equation:

$$\int \frac{dx}{\sqrt{\alpha + \beta x + \gamma x^2}} = \frac{1}{\sqrt{-\gamma}}\text{acos}[-(\beta + 2\gamma x)/\sqrt{q}] \text{ with } q = \beta^2 - 4\alpha\gamma. \tag{4.26}$$

Using this formula allows us to solve the integral in Eq. (4.25) by identifying $\alpha = 2mE/l^2$ and so forth. We obtain

$$\theta = -\text{acos}\Big[\frac{l^2/(mkr) - 1}{\sqrt{1 + 2El^2/mk^2}}\Big] \tag{4.27}$$

We can tidy up this expression quite a bit by introducing some useful parameters. First, we define the eccentricity of the orbit via

$$\epsilon = \sqrt{1 + \frac{2El^2}{mk^2}}. \tag{4.28}$$

Next, we introduce the so-called orbit parameter $p = l^2/mk$. In this way, we may rewrite the above to:

$$\theta = -\text{acos}[(p/r - 1)/\epsilon]. \tag{4.29}$$

Straight-forward algebraic manipulation of this expression yields the final answer for $r = r(\theta)$, describing the trajectory of a particle moving in a Kepler potential:

$$r = \frac{p}{1 + \epsilon\cos\theta}. \tag{4.30}$$

As announced earlier, we see that $\theta = 0$ indeed corresponds to $r = r_{\text{min}} = p/(1 + \epsilon)$ which is the perihelion of the orbit.

The question is now: what does the trajectory described by Eq. (4.30) really look like? We may distinguish between four scenarios, in complete analogy with how we distinguished between particle trajectories depending on the energy E of the particle in a previous section. We find that

- $\epsilon > 1$ (which corresponds to $E > 0$): hyperbola.
- $\epsilon = 1$ ($E = 0$): parable
- $\epsilon < 1$ ($E < 0$): ellipse
- $\epsilon = 0$ ($E = -mk^2/2l^2$): circle

Let's have a closer look at the case of an elliptical trajectory.

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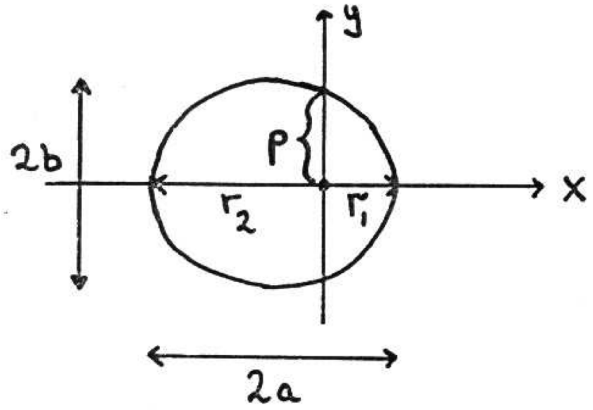

The major half-axis is denoted a while the minor one is denoted b. The motion is bound since r lies between r_1 and r_2. It follows from the figure that:

$$2a = r_1 + r_2 = p/(1+\epsilon) + p/(1-\epsilon) = 2p/(1-\epsilon^2). \tag{4.31}$$

Inserting the expressions for p and ε that we identified earlier, one arrives at

$$a = \frac{k}{2|E|}. \tag{4.32}$$

The absolute value sign comes from the fact that E is negative. Similarly, one may identify

$$b = \frac{l}{\sqrt{2m|E|}} \tag{4.33}$$

by using that the eccentricity ϵ satisfies $\epsilon = c/a$ where $2c$ is the distance between the focal points and that $a^2 = b^2 + c^2$ for an ellipse.

With these considerations, we are now in a position to establish a useful relation between the period of orbit T and the size of the elliptical trajectory. We have previously shown that the "areal velocity" is constant:

$$\frac{dA}{dt} = \frac{l}{2m} \rightarrow A = \frac{l}{2m}T \tag{4.34}$$

by integrating over one period T. For an ellipse, we have $A = \pi ab$. Inserting the above expressions we derived for a and b, we end up with

$$T = 2\pi a^{3/2}\sqrt{m/k}. \tag{4.35}$$

This is Kepler's third law, namely that $T^2 \sim a^3$.

F. Scattering cross section

In order to define what the scattering cross section is and what it gives us information about, consider a scenario where we have a uniform flux of particles heading toward the center of some potential $V(r)$. These "particles" could in reality be anything: electrons, α-particles, planets, so the situation at hand is quite general. Assume for simplicity that all particles have the same mass and energy. The potential $V(r)$ is such that the resulting force $f(r) = -\partial V/\partial r \rightarrow 0$ when $r \rightarrow \infty$. We may characterize the incident flux of particles with the intensity I:

$I =$ the number of particles passing through a unit of cross sectional area normal to the current flow per unit of time. (4.36)

The trajectory of the particles will be deflected from rectilinear motion when they get close to the center of the potential $V(r)$ since it acts with a force on them. After the particles have passed through the potential, the force acting on them subsides and their trajectories eventually return to rectilinear motion again.

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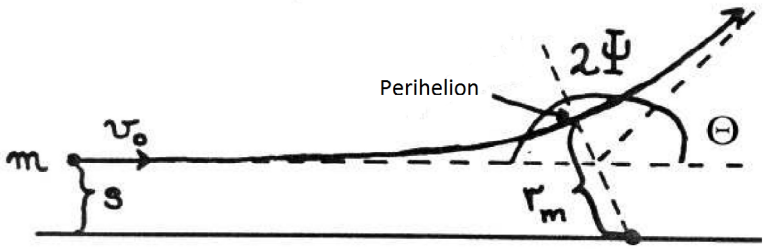
Based on the above scenario, we now define the differential scattering cross section $\sigma(\Omega)$:

$$\sigma(\Omega)\mathrm{d}\Omega = \frac{\#\text{ particles scattered into solid angle d}\Omega\text{ per unit time}}{\text{intensity of the incident flux of particles}} \tag{4.37}$$

Recall that for a solid angle, we have $\mathrm{d}\Omega = \sin\theta \mathrm{d}\theta\mathrm{d}\phi$. The unit of $\sigma(\Omega)$ thus becomes m^2. If we are dealing with central forces where the potential only depends on the absolute value of the distance from the potential center, i.e. $V(\boldsymbol{r}) = V(r)$, there exists a symmetry around the axis that defines the direction of incidence. In effect, we can integrate over $\mathrm{d}\phi$ and consider $\mathrm{d}\Omega = 2\pi \sin\theta \mathrm{d}\theta$ where θ is the scattering angle.



Let us consider a specific example where $V(r)$ is repulsive. It is convenient to introduce the impact parameter s:

$$l = |\boldsymbol{r} \times \boldsymbol{p}| =_{r\to\infty}= mv_0 s = s\sqrt{2mE}. \tag{4.38}$$

For a fixed energy E and s, the scattering angle θ will be uniquely determined. Assume then that different values of s give rise to different scattering angles θ for the incident particles. We may then state the number of particles incident between s and $s + \mathrm{d}s$ must equal the number of particles scattered between θ and $\theta + \mathrm{d}\theta$. Expressed mathematically, this gives:

$$2\pi I s|ds| = 2\pi\sigma(\theta) I \sin\theta |d\theta|. \tag{4.39}$$

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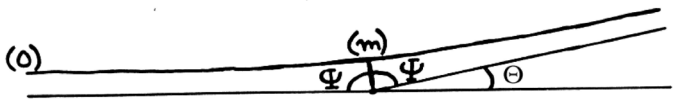
We have inserted absolute value signs due to the fact that one often has $ds/d\theta < 0$. This can be understood by noting that *decreasing* s, i.e. causing the particles to pass closer to the potential center, is likely to *increase* the scattering angle θ since they feel a stronger force. We thus end up with

$$\sigma(\theta) = \frac{s}{\sin\theta}\left|\frac{ds}{d\theta}\right|. \tag{4.40}$$

In order to find $\sigma(\theta)$, we have to find out how s and θ depend on each other in order to compute $ds/d\theta$. We can do this by going back to our previous relation between the angle of the trajectory and the radius of the trajectory that we used in our treatment of the Kepler potential. Since we already used θ for the scattering angle, so let us use β for the angle denoting a specific point on the trajectory. We have

$$\beta = \int_{r_0}^{r} \frac{dr}{r^2\sqrt{2mE/l^2 - 2mV/l^2 - 1/r^2}}. \tag{4.41}$$



From the figure, we see that $\theta + 2\psi = \pi$. Now, $r_0 = \infty$ corresponds to $\beta_0 = \pi$. Also, $r = r_m$ (the minimum radius of the trajectory, the so called *perihelion*) corresponds to $\beta = \pi - \psi$. Using these relations in the general expression Eq. (4.41), we obtain

$$(\pi - \psi) - \pi = \int_{\infty}^{r_m} \frac{dr}{r^2\sqrt{\dots}} \tag{4.42}$$

Rewriting this in terms of $s = l/\sqrt{2mE}$, we get:

$$\psi = \int_{r_m}^{\infty} \frac{s\mathrm{d}r}{r^2\sqrt{1 - V/E - s^2/r^2}}. \tag{4.43}$$

Substituting $u = 1/r$, we finally obtain the desired result which allows us to evaluate $ds/d\theta$:

$$\theta(s) = \pi - 2\int_{0}^{u_m} \frac{s\mathrm{d}u}{\sqrt{1 - V/E - s^2u^2}}. \tag{4.44}$$

Note that so far, we have not specified what the precise form of the potential V is and hence our result is generic. If V is a complicated function of r, then the above equation can only be evaluated numerically. Note that u_m is a known quantity: it is given by

$$1 - V(u_m)/E - s^2u_m^2 = 0. \tag{4.45}$$

This may be understood by noting that

$$dr = r^2\frac{\sqrt{2mE}}{l}\sqrt{1 - V/E - s^2/r^2}d\beta \tag{4.46}$$

and in the perihelion, we have $dr/d\beta = 0$ by definition. Let's have a look at an example where the trajectory can be computed analytically, so that we obtain an explicit expression for $s(\theta)$ and finally $\sigma(\theta)$.

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Example 13. Repulsive scattering between charged particles in the Coulomb-field. Consider positively charged particles with charges Ze and $Z'e$, respectively.

If $M \gg m$, the center of mass will essentially coincide with the location of M. We thus assume that particle M is at rest in our reference frame (the lab system). The Coulomb force is $f(r) = ZZ'e^2/(4\pi\epsilon_0 r^2)$ and the Coulomb potential is $V(r) = ZZ'e^2/(4\pi\epsilon_0 r)$. This is precisely the situation considered in the Kepler problem if we define $k = -ZZ'e^2/(4\pi\epsilon_0)$. We have

$$E = T + V = \frac{1}{2}mv^2 + V(r) > 0. \tag{4.47}$$

Due to conservation of energy, we also have $E = \frac{1}{2}mv_0^2$ since when the particles are far apart the only energy in the problem is the kinetic energy of particle m. Based on our previous analysis, we can immediately state that the resulting trajectory of particle m will be a hyperbola with eccentricity

$$\epsilon = \sqrt{1 + \frac{2El^2}{mk^2}} = \sqrt{1 + \frac{2El^2}{m}\left(\frac{4\pi\epsilon_0}{ZZ'e^2}\right)^2} > 1. \tag{4.48}$$

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Note that since $l^2 = 2s^2mE$. We can also see from our previous analysis of the Kepler problem that, generally, we have:

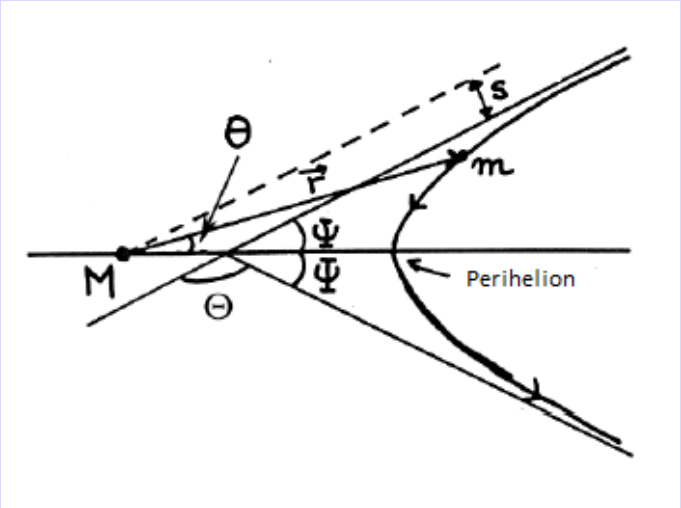
$$p/r = 1 + \epsilon\cos(\beta - \beta_0). \tag{4.49}$$

For the case of an elliptical trajectory, we saw that choosing $\beta_0 = 0$ corresponded to measuring β from the perihelion. Also, we had defined $p = l^2/mk$. In our case, we have $k < 0$ and hence $p < 0$. This has the consequence that we have to choose $\beta_0 = \pi$ in order for $\beta = 0$ to be the perihelion. We obtain

$$|p|/r = \epsilon\cos\beta - 1 \tag{4.50}$$

or alternatively:

$$r = \frac{|p|}{\epsilon\cos\beta - 1}. \tag{4.51}$$



The asymptotes of the trajectory are for $r \to \infty$:

$$\beta \to \pm\psi \tag{4.52}$$

which means that $\cos\psi = 1/\epsilon$. The scattering angle is $\theta = \pi - 2\psi$. This means that

$$\cos(\pi/2 - \theta/2) = \frac{1}{\epsilon} \tag{4.53}$$

We can rewrite this expression as

$$\cot(\theta/2) = 4\pi\epsilon_0\frac{2Es}{ZZ'e^2}. \tag{4.54}$$

and isolate s from this equation:

$$s = s(\theta, E) = \frac{1}{4\pi\epsilon_0}\frac{ZZ'e^2}{2E}\cot(\theta/2). \tag{4.55}$$

Differentiating, we obtain

$$\left|\frac{ds}{d\theta}\right| = \frac{1}{4\pi\epsilon_0}\frac{ZZ'e^2}{4E}\frac{1}{\sin^2(\theta/2)}. \tag{4.56}$$

We may then finally write down the result for the differential scattering cross section analytically:

$$\sigma(\theta) = \frac{s}{\sin\theta}\left|\frac{ds}{d\theta}\right| = \left(\frac{1}{4\pi\epsilon_0}\right)^2\left(\frac{ZZ'e^2}{4E}\right)^2\frac{1}{\sin^4(\theta/2)}. \tag{4.57}$$

This is known as Rutherfords scattering cross section. Interestingly, a fully quantum mechanical calculation (albeit non-relativistic) would yield exactly the same answer.

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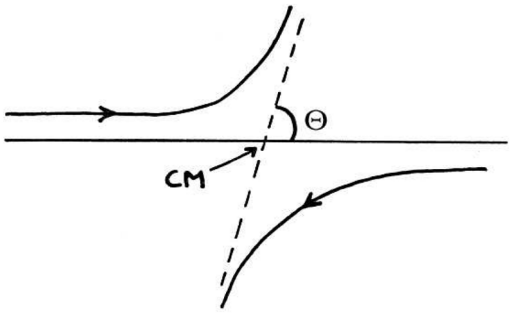
Once we have computed the differential scattering cross section, we can obtain the total scattering cross section σ as follows:

$$\sigma = \int \sigma(\Omega) d\Omega = 2\pi \int_0^\pi \sigma(\theta) \sin\theta d\theta. \tag{4.58}$$

The total cross section σ can be though of the net area that particles can be scattered into. With the Coulomb-potential, one finds that $\sigma \to \infty$. The physical interpretation of this is that the Coulomb force has an infinite range, and so regardless of how large the impact parameter s is, the particle will be scattered and contribute to σ. Quantum mechanically, one would find that if $V \to 0$ faster than $1/r^2$ when $r \to \infty$, σ will be finite.

It is also worth emphasizing that we assumed $M \gg m$ so that the center of mass was at rest. Rutherfords formula is always valid in the CM-frame if one interprets θ_{CM} as the angle between the incident and outgoing particle. In the lab-system, the angle between incident and outgoing particle will in general be different from θ_{CM}.



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V. KINEMATICS AND EQUATIONS OF MOTION FOR RIGID BODIES

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Learning goals. After reading this chapter, the student should:

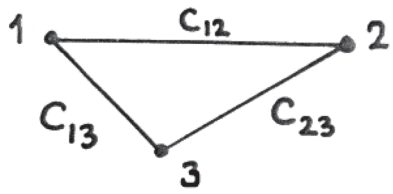
- Know about the transformation matrix
- Know how the Euler angle can be used to determine the spatial orientation of axes in a rigid body.
- Be familiar with infinitesimal transformations.
- Be familiar with the Coriolis force.

We will in this chapter consider rigid bodies, subject to the holonomic constraints that the distance between two arbitrary material points is always the same. The rigid body is in a strict sense an idealized model (it cannot exist in quantum mechanics, not even at zero absolute temperature, because of the zero-point oscillations). But it is a very useful model nevertheless. We will here deal with the *kinematics* of rigid bodies, i.e., how to specify the nature and the characteristics of their motion. The *dynamics* of rigid bodies is something different and will be considered later in this chapter: it concerns the motions as determined by the action of extraneous forces. That is, the equations of motion will then have to be taken into account.

How many degrees of freedom has a rigid body, i.e., how many coordinates are needed to specify its position? Neglecting all constraints to begin with, the body consisting of N particles has $3N$ degrees of freedom in all. This number is strongly reduced because of the constrains saying that the distance r_{ij} between particles *i* and *j* is fixed, $r_{ij} = c_{ij} = \text{constant}$. The number of these constraints is $1+2+...+N = \frac{1}{2}(N-1)$, but these are not all independent. Actually, we need only determine the position of three specified points (not lying along the same line), plus the corresponding constraints $r_{ij} = c_{ij}$. The three points are linked by three constraints of this type, so that the number of degrees of freedom is reduced from 9 to 6. With reference to the figure, consider the following simple reasoning:

- We need 3 coordinates to specify the location of one point, say point 1;
- Then we need two coordinates to specify point 2 (this point can lie on a spherical surface centered in point 1, with radius r_{12});
- We finally need one more coordinate to specify point 3 (this point can lie on a circle around the axis between 1 and 2).

. This adds up to 3+2+1=6 degrees of freedom in all.



A. Orthogonal transformations and independent coordinates

Let now x, y, z be the axes in a fixed "external" (lab) coordinate system and let x', y', z' be the corresponding axes in a coordinate system which is fixed in the rigid body. In addition to the three coordinates needed to specify the origin in the (x', y', z') system relative to the (x, y, z) system we need the *directions* of x', y' relative to x, y, z. It is convenient to use the direction cosines $\alpha_1, \alpha_2, \alpha_3$ of the primed axes relative to the unprimed. They are defined via

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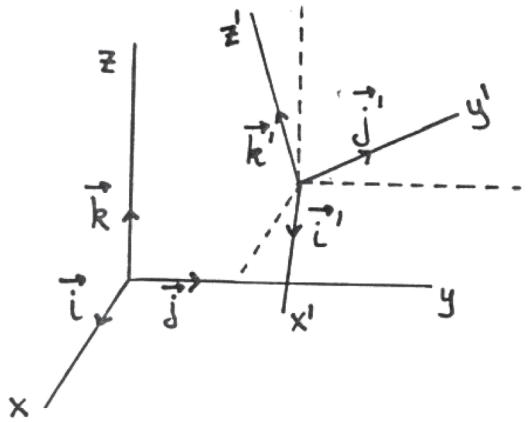

$$\begin{array}{rcccl} \alpha_1 & = & \cos(\mathbf{i}', \mathbf{i}) & = & \mathbf{i}' \cdot \mathbf{i} \\ \alpha_2 & = & \cos(\mathbf{i}', \mathbf{j}) & = & \mathbf{i}' \cdot \mathbf{j} \\ \alpha_3 & = & \cos(\mathbf{i}', \mathbf{k}) & = & \mathbf{i}' \cdot \mathbf{k} \end{array}$$

and analogous behavior with β for $\mathbf{j}'$ and γ for $\mathbf{k}'$. Since

$$\mathbf{i}' = (\mathbf{i}' \cdot \mathbf{i})\mathbf{i} + (\mathbf{i}' \cdot \mathbf{j})\mathbf{j} + (\mathbf{i}' \cdot \mathbf{k})\mathbf{k},$$

we have then

$$\boxed{\begin{array}{rcccccl} \mathbf{i}' & = & \alpha_1\mathbf{i} & + & \alpha_2\mathbf{j} & + & \alpha_3\mathbf{k} \\ \mathbf{j}' & = & \beta_1\mathbf{i} & + & \beta_2\mathbf{j} & + & \beta_3\mathbf{k} \\ \mathbf{k}' & = & \gamma_1\mathbf{i} & + & \gamma_2\mathbf{j} & + & \gamma_3\mathbf{k} \end{array}} \tag{5.1}$$

We can of course invert his process, that means, express $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ in terms of their components along $\mathbf{i}'$, $\mathbf{j}'$ and $\mathbf{k}'$:

$$\mathbf{i} = (\mathbf{i} \cdot \mathbf{i}')\mathbf{i}' + (\mathbf{i} \cdot \mathbf{j}')\mathbf{j}' + (\mathbf{i} \cdot \mathbf{k}')\mathbf{k}' = \alpha_1\mathbf{i}' + \beta_1\mathbf{j}' + \gamma_1\mathbf{k}'$$

and so on.

The direction cosines give the connection between arbitrary vectors in the two systems (x, y, z) and (x', y', z') (we assume the same origins in the two systems). For example, a position vector $\vec{r}$ will have an x'-component given by

$$x' = \mathbf{r} \cdot \mathbf{i}' = (x\mathbf{i} + y\mathbf{j} + z\mathbf{k}) \cdot \mathbf{i}' = \alpha_1 x + \alpha_2 y + \alpha_3 z,$$

and an arbitrary vector $\mathbf{G}$ will have an y'-component

$$G_{y'} = \mathbf{G} \cdot \mathbf{j}' = (G_x\mathbf{i} + \mathbf{G_y}\mathbf{j} + \mathbf{G_z}\mathbf{k}) \cdot \mathbf{j}' = \beta_1\mathbf{G_x} + \beta_2\mathbf{G_y} + \beta_3\mathbf{G_z}.$$

We have 9 direction cosines, but have seen that we need only 3 coordinates to determine the body's orientation uniquely. The reduction can be done via the orthogonality conditions:

$$\begin{aligned} \mathbf{i} \cdot \mathbf{i} &= (\alpha_1\mathbf{i}' + \beta_1\mathbf{j}' + \gamma_1\mathbf{k}')^2 = \alpha_1^2 + \beta_1^2 + \gamma_1^2 = 1 \\ \mathbf{i} \cdot \mathbf{j} &= (\alpha_1\mathbf{i}' + \beta_1\mathbf{j}' + \gamma_1\mathbf{k}') \cdot (\alpha_2\mathbf{i}' + \beta_2\mathbf{j}' + \gamma_2\mathbf{k}') = \alpha_1\alpha_2 + \beta_1\beta_2 + \gamma_1\gamma_2 = 0, \end{aligned}$$

etc. On a compact form:

$$\boxed{\alpha_l\alpha_m + \beta_l\beta_m + \gamma_l\gamma_m = \delta_{lm}} \tag{5.2}$$

We can thus *not* use the direction cosines as generalized coordinates, for instance in a Lagrangian formulation, as they are not independent. (Later, we shall see that there are three independent independent functions of the direction cosines, called the Euler angles, which can be used for this purpose.) The direction cosines are yet useful, as they describe the relationship between Cartesian coordinate systems.

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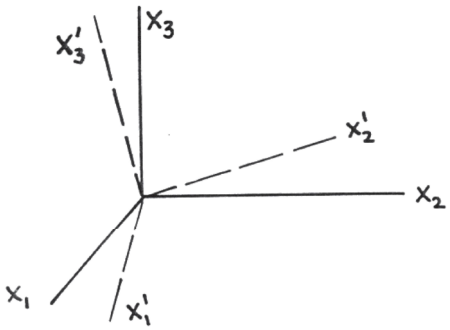
B. Transformation matrix and its mathematical properties

We introduce now a more convenient notation by letting $x, y, z \rightarrow x_1, x_2, x_3$. The transformations then become



$$\begin{aligned} x_1' &= \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 \\ x_2' &= \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 \\ x_1' &= \gamma_1 x_1 + \gamma_2 x_2 + \gamma_3 x_3 \end{aligned}$$

This is a *linear* transformation which in general can be written

$$\begin{aligned} x_1' &= a_{11} x_1 + a_{12} x_2 + a_{13} x_3 \\ x_2' &= a_{21} x_1 + a_{22} x_2 + a_{23} x_3 \\ x_3' &= a_{31} x_1 + a_{32} x_2 + a_{33} x_3, \end{aligned}$$

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where a_{ij} are *constant coefficients* (i.e., independent of x,x'). Introducing the summation convention, implying that repeated indices are to summed over, we can express this as

$$x'_i = a_{ij}x_j, \qquad i \in \{1,2,3\}. \tag{5.3}$$

The length of the vector $\boldsymbol{r}$ cannot be influenced by the transformation as it corresponds to a spatial rotation; thus

$$x'_i x'_i = x_i x_i \Rightarrow a_{ij}a_{ik}x_j x_k = x_i x_i$$

which gives

$$a_{ij}a_{ik} = \delta_{jk} \tag{5.4}$$

By inserting α, β, γ, we see that this is just the earlier 6 conditions from equation We define the rotation matrix as

$$\mathbb{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix},$$

with matrix elements a_{ij}.

Example 14. Example Two dimensions In two dimensions the transformation matrix is

$$\mathbb{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}.$$

and the orthogonality conditions are

$$a_{ij}a_{ik} = \delta_{jk}$$

With four matrix elements and three orthogonality conditions we are left with one independent variable which is naturally interpreted as the rotation angle φ. From the geometry we have

$$\begin{aligned} x'_1 &= x_1\cos\varphi + x_2\sin\varphi \\ x'_2 &= -x_1\sin\varphi + x_2\cos\varphi \end{aligned}$$

which means

$$\begin{aligned} a_{11} = \cos\varphi, &\quad a_{12} = \sin\varphi \\ a_{21} = -\sin\varphi, &\quad a_{22} = \cos\varphi \end{aligned}$$

Then

$$\mathbb{A} = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix}$$

We may check the orthogonality:

$$\begin{aligned} a_{11}a_{11} + a_{21}a_{21} &= 1 \implies & \cos^2\varphi + \sin^2\varphi &= 1 \\ a_{12}a_{12} + a_{22}a_{22} &= 1 \implies & \sin^2\varphi + \cos^2\varphi &= 1 \\ a_{11}a_{12} + a_{21}a_{22} &= 0 \implies & \cos\varphi\sin\varphi - \sin\varphi\cos\varphi &= 0 \end{aligned}$$

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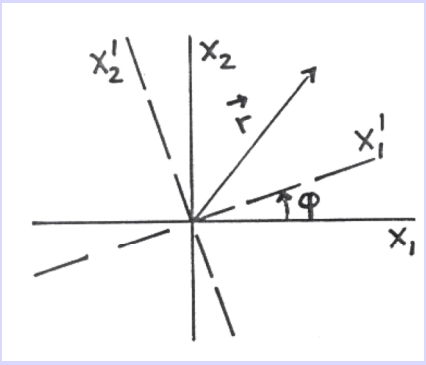
which is seen to be satisfied.



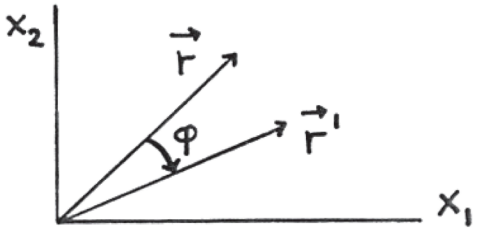
As a general point we observe that the transformation equation $\vec{r}' = \mathbb{A}\vec{r}$ can be considered in two different ways:

1. **Passive transformation**: $\mathbb{A}$ is looked upon as an operator that rotates the *coordinate system* (counterclockwise in the example above), while the vector $\vec{r}$ itself is unchanged. We find thus the components of $\vec{r}$ in the rotated coordinate system. As we will see, this is the usual way of looking at transformations in special relativity, as Lorentz transformations can be pictured as rotations in a four-dimensional spacetime.
2. **Active transformation**: $\mathbb{A}$ is looked upon as an operator that rotates the *vector* $\vec{r}$, while the coordinate system is unchanged. We thus find a new vector $\vec{r}'$ in the same coordinate system as before (we must rotate the vector clockwise in order to get the same equations $\vec{r}' = \mathbb{A}\vec{r}$ as above). This is a way of interpretation often used in quantum field theory.

C. Formal properties of the transformation matrix

Let us look at two successive transformations:

$$\vec{r} \underbrace{\longrightarrow \vec{r}'}_{\mathbb{B}} \underbrace{\longrightarrow \vec{r}''}_{\mathbb{A}}$$



With use of the summation convention we can write this as

$$\begin{aligned} x_k' &= b_{kj}x_j \\ x_i'' &= a_{ik}x_k' \\ &\Downarrow \\ x_i'' &= a_{ik}b_{kj}x_j \equiv c_{ij}x_j; \qquad c_{ij} = a_{ik}b_{kj} \end{aligned}$$

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We thus see that two orthogonal transformations $\mathbb{A}$ and $\mathbb{B}$ following each other are equivalent to one transformation $\mathbb{C}$ such that $\mathbb{C} = \mathbb{AB}$. It can be verified that also $\mathbb{C}$ is an orthogonal transformation. In general one has

$$\mathbb{AB} \neq \mathbb{BA}$$

so that the transformation is **non-commutative**. Further, one has

$$(\mathbb{AB})\mathbb{C} = \mathbb{A}(\mathbb{BC}),$$

showing that the transformation is **associative**.

So far, we have dealt with quadratic matrices. We now introduce column matrices:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \qquad \mathbf{x}' = \begin{bmatrix} x_1' \\ x_2' \\ x_3' \end{bmatrix}.$$

The matrix $\mathbb{A}\mathbf{x}$ becomes therewith a column matrix with elements $(\mathbb{A}\mathbf{x})_i = a_{ij}x_j = x_i' = (x')_i$, that means,

$$\mathbf{x}' = \mathbb{A}\mathbf{x}.$$

Note that we have not done anything else than writing the vector $\vec{r}$ as a column matrix $\mathbf{x}$, where the number of elements is the same as the dimensionality of the space under consideration.

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The inverse transformation is written as $\mathbb{A}^{-1}$, with matrix elements a_{ij}^{-1} [note: a_{ij}^{-1} is the (i,j)-element of $\mathbb{A}^{-1}$, *not* "$1/a_{ij}$"!]. The transformation $\mathbb{A}^{-1}$ shall bring $\mathbf{x}$ back to $\mathbf{x}$:

$$\begin{aligned} x_i &= a_{ij}^{-1} x'_j \\ \Rightarrow x'_k &= a_{ki} x_i = a_{ki} a_{ij}^{-1} x'_j \\ \Rightarrow \underbrace{a_{ki} a_{ij}^{-1}}_{(\mathbb{A}\mathbb{A}^{-1})_{kj}} &= \underbrace{\delta_{kj}}_{\mathbb{I}_{kj}} \end{aligned}$$

thus:

$$\mathbb{A}\mathbb{A}^{-1} = \mathbb{I}$$

where $\mathbb{I}$ is the unit matrix, also called the Kronecker symbol. In three spatial dimensions it reads

$$\mathbb{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

From $x_i = a_{ij}^{-1} x'_j = a_{ij}^{-1} a_{jk} x_k$ we get $a_{ij}^{-1} a_{jk} = \delta_{ik}$, i.e., $\mathbb{A}^{-1}\mathbb{A} = \mathbb{I}$, which means

$$\boxed{\mathbb{A} \text{ and } \mathbb{A}^{-1} \text{ commute}} \tag{5.5}$$

Now consider the double sum $a_{kl} a_{ki} a_{ij}^{-1}$. By using the orthogonality conditions $a_{kl} a_{ki} = \delta_{il}$ we see that this becomes equal to a_{lj}^{-1}. Alternatively, we can exploit that $a_{ki} a_{ij}^{-1} = \delta_{kj}$ to see that the double sum can also be written as a_{jl}. Accordingly, $a_{lj}^{-1} = a_{jl}$. But $a_{jl} = \tilde{a}_{lj}$, thus the (l,j)-element of the **transposed matrix** $\tilde{\mathbb{A}}$. This means that

$$\boxed{\mathbb{A}^{-1} = \tilde{\mathbb{A}} \text{ and } \tilde{\mathbb{A}}\mathbb{A} = \mathbb{I} \text{ for orthogonal matrices}} \tag{5.6}$$

Again using the summation convention we write $\tilde{\mathbb{A}}\mathbb{A} = \mathbb{I} \Rightarrow \tilde{a}_{ij} a_{jk} = \delta_{ik}$ and $\mathbb{A}\tilde{\mathbb{A}} = \mathbb{I} \Rightarrow a_{ij} \tilde{a}_{jk} = \delta_{ik}$, so that

$$\begin{aligned} a_{ji} a_{jk} &= \delta_{ik} \qquad \text{sum over first index} \\ a_{ij} a_{kj} &= \delta_{ik} \qquad \text{sum over second index} \end{aligned} \tag{5.7}$$

Finally, we consider the determinant $|\mathbb{A}|$ of the (assumed quadratic) matrix $\mathbb{A}$ (the symbol $||$ means the determinant, not the modulus!). From courses in mathematics we know that

$$|\mathbb{A}\mathbb{B}| = |\mathbb{A}| \cdot |\mathbb{B}|.$$

Since $\tilde{\mathbb{A}}\mathbb{A} = \mathbb{I}$, one has $|\tilde{\mathbb{A}}| \cdot |\mathbb{A}| = 1$, and as the value of the determinant does not depend on the interchange between the interchange $\leftrightarrow$ columns, we get $|\tilde{\mathbb{A}}| = |\mathbb{A}|$, and therewith

$$|\mathbb{A}|^2 = 1 \text{ for all orthogonal matrices} \tag{5.8}$$

This implies that $|\mathbb{A}| = e^{i\theta}$, with $0 \leq \theta \leq 2\pi$. If $|\mathbb{A}|$ is a real quantity, we get $|\mathbb{A}| = \pm 1$.

D. Euler angles

We found above that the 9 a_{ij} cannot serve as independent coordinates since a rotating body with one point fixed can have only 3 degrees of freedom. By means of 6 orthogonality conditions we managed to reduce the number of coordinates to the right number of 3. In addition we have always one extra condition, namely that the transformation shall be possible physically. This implies that the rotation matrix goes continuously over to the unit matrix, corresponding to no rotation at all, when the rotation angle goes to zero. Mathematically, this means that $|\mathbb{A}| = |\mathbb{I}| = +1$. We *cannot* have $|\mathbb{A}| = -1$ if the transformation shall be physically realizable.

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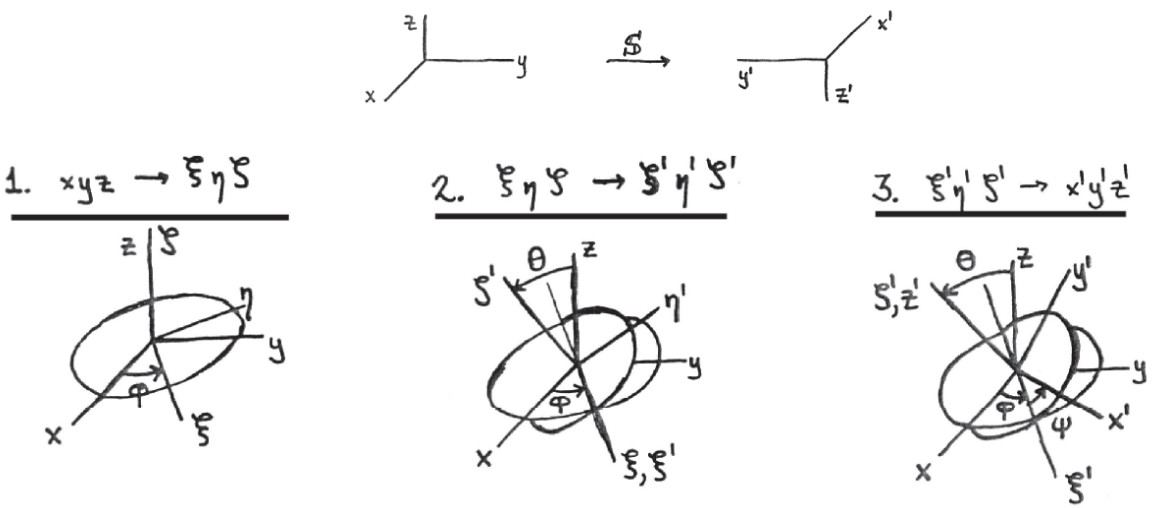
As a simple example we may consider the matrix

$$\mathbb{S} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

which implies a reflection of the coordinate axes: $\mathbf{x}' = \mathbb{S}\mathbf{x} \Rightarrow x' = -x, y' = -y, z' = -z$. This transformation is excluded, as is reasonable also from the fact that $\mathbb{S}$ changes a right-handed coordinate system into a left-handed one.
We have to find 3 independent coordinates necessary to fix the orientation of the rigid body, in such a way that the orthogonal transformation matrix $\mathbb{A}$ satisfies $|\mathbb{A}| = +1$. The most common choice is to introduce the so-called Euler angles. The transformation consists in three successive rotations involving three angles, called ϕ, θ, ψ, in a specifies order:



1. $xyz \to \xi\eta\zeta$ by a rotation an angle ϕ in a positive (counterclockwise) direction around the z-axis. Thus $\mathbf{x}'' = \mathbb{D}\mathbf{x}$, with $\mathbf{x}'' = \begin{bmatrix} \xi \\ \eta \\ \zeta \end{bmatrix}, \mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$.
2. $\xi\eta\zeta \to \xi'\eta'\zeta'$ by a rotation an angle θ in positive (counterclockwise) direction about the ξ-axis. The ξ-axis is called the line of nodes. Thus $\mathbf{x}''' = \mathbb{C}\mathbf{x}''$, with $\mathbf{x}''' = \begin{bmatrix} \xi' \\ \eta' \\ \zeta' \end{bmatrix}$.
3. $\xi'\eta'\zeta' \to x'y'z'$ by a rotation an angle ψ in positive (counterclockwise) direction about the ζ'-axis. Thus $\mathbf{x}' = \mathbb{B}\mathbf{x}'''$, $\mathbf{x}' = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}$.

Let us consider in more detail $\mathbb{D}$, the first of the three transformation matrices. It describes a rotation about the z-axis:

$$\mathbb{D} = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{5.9}$$

The reason for the number '1' in the lower right corner is that it specifies which axis the rotation takes place about. In this way we manage to describe an initial two-dimensional rotation in a three-dimensional space.

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The second matrix describes the rotation about the ξ-axis (the line of nodes):

$$\mathbb{C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}, \tag{5.10}$$

where the number '1' in the upper left corner specifies that in this case the rotation axis is the line of nodes.

Finally, the matrix $\mathbb{B}$ describes the rotation about the ζ'-axis:

$$\mathbb{B} = \begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{5.11}$$

where evidently the '1' to the lower right refers to the ζ'-axis.

The composite transformation $\mathbb{A}$ is built up from these elementary matrices,

$$\mathbb{A} = \mathbb{B}\mathbb{C}\mathbb{D}, \tag{5.12}$$

where the equation is to be read from right to left. Multiplying out the matrices we get the general form

$$\mathbb{A} = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\theta & -\sin\psi\sin\phi - \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix} \tag{5.13}$$

The inverse transformation $\mathbf{x} = \mathbb{A}^{-1}\mathbf{x}'$ is given by $\mathbb{A}^{-1} = \tilde{\mathbb{A}}$, which follows by interchanging lines and columns in $\mathbb{A}$.

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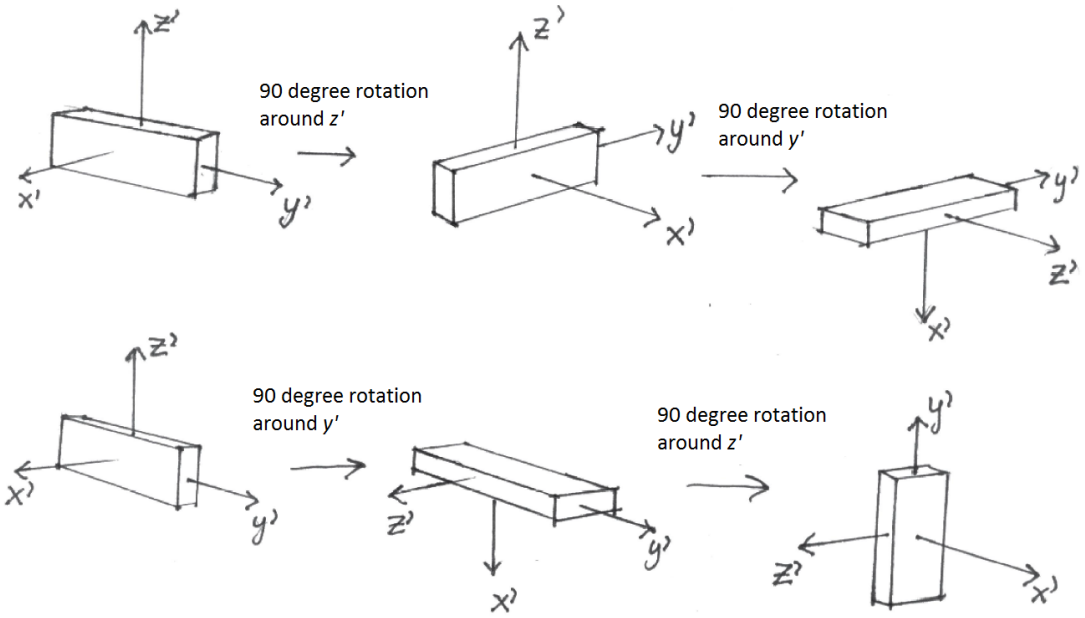
E. Infinitesimal transformations

Two successive transformations can be described as a product of two matrices, $\mathbb{AB}$. We know that matrix multiplication is in general non-commutative, i.e. $\mathbb{AB} \neq \mathbb{BA}$. This is illustrated by an example shown in the figure, where a rectangular box is subject to two rotations, but in different order .



So far, we have considered finite transformations. We shall now see that, in contradistinction to most finite transformations, **infinitesimal transformations** are commutative. Consider, on tensor form, the infinitesimal transformation

$$x_i' = x_i + e_{ij}x_j = (\delta_{ij} + e_{ij})x_j, \qquad |e_{ij}| \ll 1.$$

On matrix form,

$$\mathbf{x}' = (\mathbb{I} + \mathbb{E})\mathbf{x}.$$

where the matrix $\mathbb{E}$ is composed of the elements e_{ij}. Now consider two successive transformations,

$$\begin{aligned}(\mathbb{I} + \mathbb{E}_1)(\mathbb{I} + \mathbb{E}_2) &= \mathbb{I} + \mathbb{E}_1\mathbb{I} + \mathbb{I}\mathbb{E}_2 + \cdots \\ &= \mathbb{I} + \mathbb{E}_1 + \mathbb{E}_2,\end{aligned}$$

since terms of second order in infinitesimal transformations can be neglected ($\mathbb{E}$ being an "infinitesimal" transformation means just that the e_{ij} are so small that $\mathcal{O}(e_{ij}^2)$ terms are negligible). As $\mathbb{I} + \mathbb{E}_1 + \mathbb{E}_2 = \mathbb{I} + \mathbb{E}_2 + \mathbb{E}_1$, we get

$$(\mathbb{I} + \mathbb{E}_1)(\mathbb{I} + \mathbb{E}_2) = (\mathbb{I} + \mathbb{E}_2)(\mathbb{I} + \mathbb{E}_1), \tag{5.14}$$

that is,

Infinitesimal transformations are commutative	(5.15)

It follows immediately that the inverse transformation is

$$\mathbb{A}^{-1} = \mathbb{I} - \mathbb{E},$$

because $\mathbb{A}\mathbb{A}^{-1} = (\mathbb{I}+\mathbb{E})(\mathbb{I}-\mathbb{E}) = \mathbb{I}$, where we again neglect terms $\mathcal{O}(e^2)$. We know from before that the transformation matrix is orthogonal,

$$\tilde{\mathbb{A}} \equiv \mathbb{I} + \tilde{\mathbb{E}} = \mathbb{A}^{-1} \Rightarrow \tilde{\mathbb{E}} = -\mathbb{E}$$
$$\Downarrow$$

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$$\tilde{e}_{ij} \equiv e_{ji} = -e_{ij}, \tag{5.16}$$

that is, the matrix $\mathbb{E}$ is antisymmetric. A general infinitesimal antisymmetric matrix has thus only three independent elements; Let us call them $d\Omega_1, d\Omega_2, d\Omega_3$. It is natural to arrange them cyclically in the matrix $\mathbb{E}$ as

$$\mathbb{E} = \begin{bmatrix} 0 & d\Omega_3 & -d\Omega_2 \\ -d\Omega_3 & 0 & d\Omega_1 \\ d\Omega_2 & -d\Omega_1 & 0 \end{bmatrix} \tag{5.17}$$

and thus

$$\begin{aligned} \mathbf{x}' - \mathbf{x} \equiv d\mathbf{x} &= \mathbb{E}\mathbf{x} \\ &= \begin{bmatrix} 0 & d\Omega_3 & -d\Omega_2 \\ -d\Omega_3 & 0 & d\Omega_1 \\ d\Omega_2 & -d\Omega_1 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}. \end{aligned}$$

On component form, with use of the summation convention, this becomes

$$dx_i = \epsilon_{ijk} x_j d\Omega_k$$

Alternatively, we can write it as

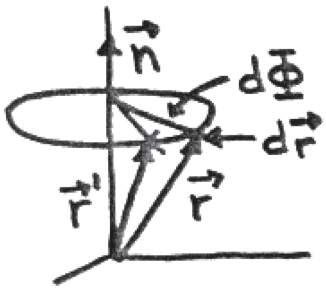
$$\boxed{d\mathbf{r} = \mathbf{r} \times d\mathbf{\Omega}.} \tag{5.18}$$

Note that the quantity $d\mathbf{\Omega}$ is a differential vector (*not* the differential of a finite vector. There exists no vector of which $d\mathbf{\Omega}$ is the differential. A *finite* rotation cannot be represented by by a single vector). Let us compare with the equations for rotation found earlier: $d\mathbf{\Omega}$ can be interpreted physically as a small vectorial change

$$d\mathbf{\Omega} = \mathbf{n} d\Phi,$$

where $d\Phi$ is a small angle. Thus

$$d\mathbf{r} = \mathbf{r} \times \mathbf{n} d\Phi$$



F. The rate of change of time-dependent vectors

Let us now use the above results to describe the rate of change of a vector. Consider a rigid body rotating with an instantaneous angular velocity $\omega = d\mathbf{\Omega}/dt$ when seen from an 'absolute' coordinate system outside the body. Such a system is also called an inertial system, characterized by the validity of Newton's ordinary equations of motion. We let such a system be designated by a subscript s. Let $\mathbf{G}$ be an arbitrary vector ($= \mathbf{r}, \mathbf{v}, \mathbf{L}$, etc.) Because of the rotation of the axes of the body, the rate of change of $\mathbf{G}$ will be perceived differently in the absolute system and in the relative (comoving) system whose axes are fixed in the body. Let quantities referring to the relative system be given a subscript 'r'.
Assume first that $\mathbf{G}$ is fixed in the body, so that $d\mathbf{G}_r = 0$. Then, we can find $d\mathbf{G}_s$ from the formula for pure rotation,

$$d\mathbf{G}_s = d\mathbf{\Omega} \times \mathbf{G}$$

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In general, $\mathbf{G}_r$ as seen in the body frame may change also. Thus we obtain as a natural generalization of the last equation,

$$d\mathbf{G}_s = d\mathbf{G}_r + d\mathbf{\Omega} \times \mathbf{G}$$

The rate of change of this quantity is

$$\left(\frac{d\mathbf{G}}{dt}\right)_s = \left(\frac{d\mathbf{G}}{dt}\right)_r + \omega \times \mathbf{G}, \tag{5.19}$$

where $\omega = d\mathbf{\Omega}/dt$ is the instantaneous angular velocity. As $\mathbf{G}$ is a general vector we can write this as an operator relation,

$$\boxed{(\tfrac{d}{dt})_s = (\tfrac{d}{dt})_r + \omega\times} \tag{5.20}$$

For example: $\mathbf{G} = \mathbf{r} \Longrightarrow \mathbf{v}_s = \mathbf{v}_r + \omega \times \mathbf{r}$.

G. Components of ω along the body axes

It is often useful to know the components of the angular velocity ω along the body axes x', y', and z'. The corresponding transformation can be taken as 3 successive rotation axes with angular velocities respectively $\omega_\phi = \dot{\phi}, \omega_\theta = \dot{\theta}$ and $\omega_\psi = \dot{\psi}$. We use the theory from above to find the components:

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- $\vec{\omega}_\phi$ corresponds to a rotation about the z-axis, i.e. $\omega_\phi = \begin{bmatrix} 0 \\ 0 \\ \dot{\phi} \end{bmatrix}$, and

$$\omega'_\phi = \mathbb{A}\,\vec{\omega}_\phi.$$

. Inserting the components of $\mathbb{A}$ found earlier we get

$$(\omega_\phi)_{x'} = \dot{\phi}\sin\theta\sin\psi, \qquad (\omega_\phi)_{y'} = \dot{\phi}\sin\theta\cos\psi, \qquad (\omega_\phi)_{z'} = \dot{\phi}\cos\theta.$$

- ω_θ corresponds to a rotation about the ξ-axis, i.e. $\omega_\theta = \begin{bmatrix} \dot{\theta} \\ 0 \\ 0 \end{bmatrix}$, and the transformation becomes

$$\omega'_\theta = \mathbb{B}\,\vec{\omega}_\theta.$$

. Inserting the components of $\mathbb{B}$ found earlier we get

$$(\omega_\theta)_{x'} = \dot{\theta}\cos\psi, \qquad (\omega_\theta)_{y'} = -\dot{\theta}\sin\psi, \qquad (\omega_\theta)_{z'} = 0$$

- As ω_ψ corresponds to a rotation about the ζ'-axis, and thus about z', is no further transformation necessary.We get simply

$$\omega'_\psi = \vec{\omega}_\psi = \begin{bmatrix} 0 \\ 0 \\ \dot{\psi} \end{bmatrix}.$$

Adding the three contributions, we get finally

$$\begin{aligned} \omega_{x'} &= \dot{\phi}\sin\theta\sin\psi + \dot{\theta}\cos\psi \\ \omega_{y'} &= \dot{\phi}\sin\theta\cos\psi - \dot{\theta}\sin\psi \\ \omega_{z'} &= \dot{\phi}\cos\theta + \dot{\psi} \end{aligned} \tag{5.21}$$

On vector form, we thus have

$$\omega = \omega_{x'}\mathbf{i}' + \omega_{y'}\mathbf{j}' + \omega_{z'}\mathbf{k}'$$

H. The Coriolis force

We go back to the operator relation $(d/dt)_s = (d/dt)_r + \omega\times$, letting subscript s refer to the absolute space as before, and letting subscript 'r' now refer to the earth as a rotating rigid body. We assume that the time dependence of ω is negligible.
We first apply the operator relation on $\mathbf{r}$, giving

$$\mathbf{v}_s = \mathbf{v}_r + \omega \times \mathbf{r}, \tag{5.22}$$

as noted above. We next apply the same operator relation on $\mathbf{r}_s$:

$$\begin{aligned} \left(\frac{d}{dt}\mathbf{v}_s\right)_s &= \left(\frac{d}{dt}\mathbf{v}_s\right)_r + \omega \times \mathbf{v}_s \\ &= \left[\frac{d}{dt}\mathbf{v}_r + \frac{d}{dt}(\omega \times \mathbf{r})\right]_r + \omega \times \mathbf{v}_r + \omega \times (\omega \times \mathbf{r}). \end{aligned}$$

As $\left[\frac{d}{dt}(\omega \times \mathbf{r})\right]_r = \omega \times \mathbf{v}_r$, we get

$$\mathbf{a}_s = \mathbf{a}_r + 2\omega \times \mathbf{v}_r + \omega \times (\omega \times \mathbf{r}) \tag{5.23}$$

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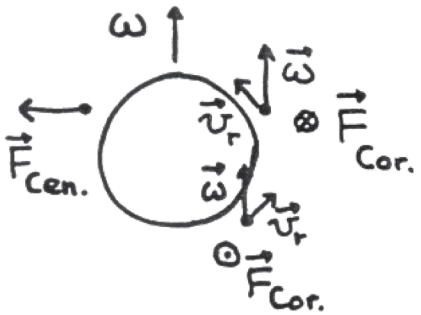
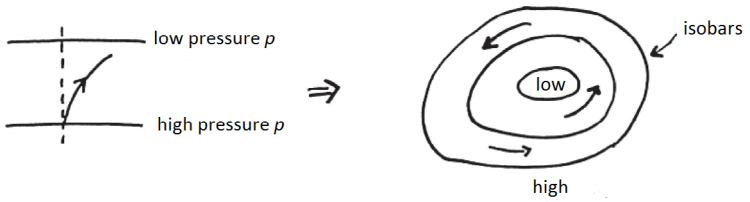
In the absolute space Newton's relations hold: $\mathbf{F} = m\mathbf{a}_s$. Thus we obtain

$$\boxed{\mathbf{F}_{\text{eff}} = m\mathbf{a}_r; \qquad \mathbf{F}_{\text{eff}} \equiv \mathbf{F} + \underbrace{2m\mathbf{v}_r \times \omega}_{\text{Coriolis force}} - \underbrace{m\omega \times (\omega \times \mathbf{r})}_{\text{Centrifugal force}}} \tag{5.24}$$

This expression shows that the Coriolis force gives a deviation to the right on the Northern hemisphere and to the left on the Southern hemisphere. The angular velocity of the earth is $\omega = 7,29 \cdot 10^{-5}\text{s}^{-1}$. Letting the axes in the earth and in the absolute space be coincident at a specified instant, we find that $r\omega^2 = 3.38\text{cm/s}^2$ is the maximal centripetal acceleration. The Coriolis force is of importance for the wind systems around the earth. Thus on the Northern hemisphere, this force tends to make the winds circulate in a counterclockwise direction around a low-pressure region.





I. Angular momentum and kinetic energy

As we have seen, we need 6 independent coordinates to describe a rigid body: a convenient choice is three spatial coordinates to fix the position of the center of mass (CM), plus three additional coordinates (the Euler angles) to specify the orientation of the body axes relative to CM. This formalism can be looked upon as a preliminary for describing the motion of the body when acted upon by extraneous forces. We may place the origin in whatever point we like, but a natural choice will often be the center of mass. Consider the rotation of a rigid body. Its angular frequency ω is the same for all points, so that it can be taken as a characteristic property of the body as a whole.
The total angular momentum about the chosen fixed point reads:

$$\mathbf{L} = \sum_i m_i(\mathbf{r}_i \times \mathbf{v}_i). \tag{5.25}$$

With a pure rotation we have $\mathbf{v}_i = \omega \times \mathbf{r}_i$, so that

$$\mathbf{L} = \sum_i m_i \mathbf{r}_i \times (\omega \times \mathbf{r}_i) = \sum_i m_i \left[\omega r_i^2 - \mathbf{r}_i(\mathbf{r}_i \cdot \omega)\right]. \tag{5.26}$$

Consider one component of $\mathbf{L}$, for example L_x:

$$\begin{aligned} L_x &= \sum_i m_i \left[\omega_x r_i^2 - x_i(x_i\omega_x + y_i\omega_y + z_i\omega_z)\right] \\ &= \sum_i m_i \left[\omega_x(r_i^2 - x_i^2) - \omega_y x_i y_i - \omega_z x_i z_i\right]. \end{aligned}$$

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Evidently we get analogous expressions for L_y and L_z, and we see that the components of $\vec{L}$ are linearly related to the components of ω. This we can express as (summation convention used)

$$L_j = I_{jk}\omega_k, \tag{5.27}$$

where I_{jk} er inertia tensor (or matrix). From the above expression for L_x we conclude that

$$I_{xx} = \sum_i m_i(r_i^2 - x_i^2)$$
$$I_{xy} = -\sum_i m_i x_i y_i$$

and so forth for the other components. With a continuously distributed mass we substitute $m_i \to \rho(\vec{r})$ and $\sum_i \to \int_V dV$, so that

$$I_{xx} = \int_V \rho(\vec{r})(r^2 - x^2)dV$$
$$I_{xy} = -\int_V \rho(\vec{r})xydV.$$

Letting $x, y, z \to x_1, x_2, x_3$ we obtain the general expression

$$\boxed{I_{jk} = \int_V \rho(\vec{r})\left(r^2\delta_{jk} - x_j x_k\right)dV} \tag{5.28}$$

With the usual notation for tensors we get the equation

$$\mathbf{L} = \mathbb{I} \cdot \omega \tag{5.29}$$

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The kinetic energy for the motion about the fixed point is

$$T = \frac{1}{2}\sum_i m_i v_i^2 = \frac{1}{2}\sum_i m_i \mathbf{v}_i \cdot \mathbf{v}_i = \frac{1}{2}\sum_i m_i \mathbf{v}_i \cdot (\omega \times \mathbf{r}_i)$$
$$= \frac{1}{2}\sum_i m_i \omega \cdot (\mathbf{r}_i \times \mathbf{v}_i) = \frac{1}{2}\omega \cdot \mathbf{L},$$

where we have used $\mathbf{v}_i = \omega \times \mathbf{r}_i$, as $(\mathbf{v}_i)_r = 0$. Using $\mathbf{L} = \mathbb{I} \cdot \omega\vec{L}$ we get

$$T = \frac{1}{2}\omega \cdot \mathbb{I} \cdot \omega \tag{5.30}$$

which can also be written as

$$T = \frac{1}{2}\omega_j I_{jk} \omega_k = \frac{1}{2} I_{jk}\omega_j\omega_k.$$

Taking $\mathbf{n}$ as the rotation axis (i.e. $\omega = \omega\mathbf{n}$), we have

$$T = \frac{1}{2} n_j \omega I_{jk} n_k \omega = \frac{1}{2}(n_j I_{jk} n_k)\omega^2 = \frac{1}{2} I\omega^2,$$

where we have defined the moment of inertia tensor around the rotation axis:

$$I \equiv n_j I_{jk} n_k = \mathbf{n} \cdot \mathbb{I} \cdot \mathbf{n}$$

From the expression for the inertia tensor we see that $I_{jk} = I_{kj}$, i.e. $\mathbb{I}$ is a symmetric matrix. Further, all components I_{jk} are real, and thus $\mathbb{I}$ becomes a **Hermitian** (self-adjoint) matrix. For a Hermitian matrix one has

$$\mathbb{A} = \mathbb{A}^\dagger \equiv (\tilde{\mathbb{A}})^*.$$

Thus, we can always *diagonalize* $\mathbb{I}$, i.e. find a coordinate system where the matrix is diagonal:

$$\mathbb{I} = \begin{bmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & I_3 \end{bmatrix},$$

where the elements are the I_1, I_2 and I_3 principal moments of inertia. We will denote the corresponding principal axes by x_1, x_2, x_3, with angular momentum components

$$L_1 = I_1\omega_1, \qquad L_2 = I_2\omega_2, \qquad L_3 = I_3\omega_3,$$

and kinetic energy

$$T = \frac{1}{2}\sum_j I_j \omega_j^2$$

For example, a symmetric spinning top has $I_1 = I_2 \neq I_3$, and a spherically symmetric top has $I_1 = I_2 = I_3 = I \Rightarrow \mathbf{L} = I\omega$.

J. The Euler equations

Let us derive the equations of motion for a rigid body rotating about a fixed point. From earlier considerations we know that the equation

$$\left(\frac{d\boldsymbol{L}}{dt}\right)_s = \boldsymbol{N},$$

holds in an inertial system, i.e. without rotation. Here, we use $\boldsymbol{N}$ for the torque in contrast to the previously used $\boldsymbol{\tau}$. We recall also the operator equation

$$\left(\frac{d}{dt}\right)_s = \left(\frac{d}{dt}\right)_r + \omega\times$$
$$\Longrightarrow \left(\frac{d\mathbf{L}}{dt}\right)_s = \left(\frac{d\boldsymbol{L}}{dt}\right)_r + \omega \times \mathbf{L},$$

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thus in the rotating system (we drop hereafter the subscripts s and r):

$$\frac{d\mathbf{L}}{dt} + \omega \times \boldsymbol{L} = \boldsymbol{N}, \tag{5.31}$$

which are the **Euler equations** on vector form when one point is fixed.

Example 15. Body axes as the principal axes Assume that the body axes are coincident with the principal axes. Then,

$$L_1 = I_1\omega_1, \qquad L_2 = I_2\omega_2, \qquad L_3 = I_3\omega_3.$$

The i-component of the Euler equation is

$$\dot{L}_i + \epsilon_{ijk}\omega_j L_k = N_i,$$

On component form this means

$$\begin{aligned} I_1\dot{\omega}_1 - \omega_2\omega_3(I_2 - I_3) &= N_1 \\ I_2\dot{\omega}_2 - \omega_3\omega_1(I_3 - I_1) &= N_2 \\ I_3\dot{\omega}_3 - \omega_1\omega_2(I_1 - I_2) &= N_3 \end{aligned}$$

K. Free rotation of rigid body; precession

We will consider a rigid body that rotates freely, and describe its precession around the rotation axis. Assume that there is no external torque, $\boldsymbol{N} = 0$. The Euler equations then give

$$\begin{aligned} I_1\dot{\omega}_1 &= \omega_2\omega_3(I_2 - I_3) \\ I_2\dot{\omega}_2 &= \omega_3\omega_1(I_3 - I_1) \\ I_3\dot{\omega}_3 &= \omega_1\omega_2(I_1 - I_2) \end{aligned}$$

There are two constants of motion, namely the kinetic energy and the angular momentum. Assume that the body is symmetric, $I_1 = I_2$. Then,

$$\begin{aligned} I_1\dot{\omega}_1 &= \omega_2\omega_3(I_1 - I_3) \\ I_1\dot{\omega}_2 &= -\omega_3\omega_1(I_1 - I_3) \\ I_3\dot{\omega}_3 &= 0. \end{aligned}$$

From the last equation we see that ω_3 is a constant, determined by the initial conditions. The two other angular frequency components ω_1 and ω_2 are determined by

$$\dot{\omega}_1 = -\Omega\omega_2, \qquad \dot{\omega}_2 = \Omega\omega_1,$$

where Ω is a new angular frequency defined as

$$\Omega = \frac{I_3 - I_1}{I_1}\omega_3.$$

We now eliminate ω_2 by combining the above equations,

$$\begin{aligned} & \ddot{\omega}_i + \Omega^2\omega_i = 0 \\ \Longrightarrow \qquad & \omega_1(t) = \omega_\perp \cos\Omega t, \qquad \omega_2(t) = \omega_\perp \sin\Omega t, \qquad \omega_\perp^2 = \omega_1^2 + \omega_2^2 \end{aligned}$$

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We see from this that the vector $\omega_1\mathbf{i} + \omega_2\mathbf{j}$ has constant magnitude and rotates (precesses) about the body's z-axis with angular frequency Ω. As ω_3 is a constant, ω has constant length and precesses about the rotation axis. The precession is relative to the body axes, which by themselves rotate with a higher angular frequency ω.

The kinetic energy is

$$T = \frac{1}{2}I_1(\omega_1^2 + \omega_2^2) + \frac{1}{2}I_3\omega_3^2 = \frac{1}{2}I_1\omega_\perp^2 + \frac{1}{2}I_3\omega_3^2 = \text{const.}$$
$$L^2 = I_1^2\omega_\perp^2 + I_3^2\omega_3^2 = \text{const.}$$

Thus $\omega_\perp$ and ω_3 can be expressed in terms of T and L. We see that if $I_1 \simeq I_3$, then $\Omega \ll \omega$.

Example 16. Rotation of the earth As is known, the earth is a little flattened at the poles (it has an oblate form), so that by letting the z-axis be the polar axis we can write $I_3 > I_1 = I_2$.

$$\Omega = \frac{I_3 - I_1}{I_1}\omega_3 \simeq \frac{1}{300}\omega_3.$$

As is moreover known,

$$\frac{2\pi}{\omega_3} = 1 \text{ day}.$$

This leads to a precession period of $\frac{2\pi}{\Omega} \simeq \frac{2\pi}{\omega_3} \cdot 300 = 300$ days. The observed period is 440 days and is called the "Chandler wobble". The deviation from the predicted period is attributed to the elastic properties of the earth; the earth is not perfectly rigid.

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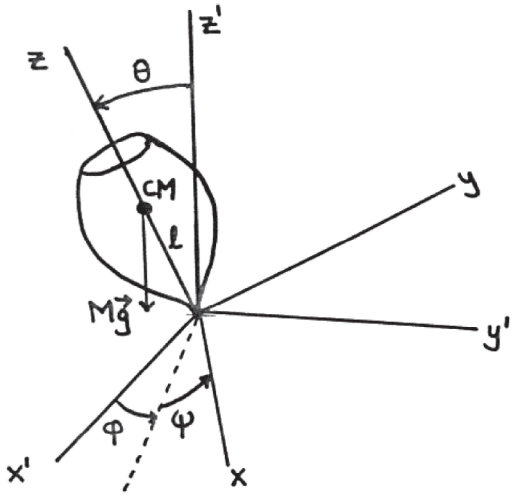
L. Heavy symmetric top with one point fixed



We consider a heavy symmetric top spinning about its principal axis in the gravitational field. The gravitational acceleration is $\boldsymbol{g}$. One point on the symmetry axis is fixed. The coordinate system $x'y'z'$ is now taken to be fixed in space so that $\boldsymbol{g} = -g\hat{z}'$, whereas xyz lies fixed in the body such that $\hat{z}$ is the symmetry axis. The geometrical symmetry implies that

$$I_1 = I_2 \neq I_3, \qquad (x_1 x_2 x_3) = (xyz).$$

The kinetic energy is

$$T = \frac{1}{2} I_j \omega_j^2 = \frac{1}{2} I_1 (\omega_1^2 + \omega_2^2) + \frac{1}{2} I_3 \omega_3^2.$$

We make use of the Euler angles ϕ, θ, ψ as (generalized) independent coordinates. From earlier we have

$$\begin{aligned} \omega_1 &= \dot{\phi} \sin\theta \sin\psi + \dot{\theta} \cos\psi \\ \omega_2 &= \dot{\phi} \sin\theta \cos\psi - \dot{\theta} \sin\psi \\ \omega_3 &= \dot{\phi} \cos\theta + \dot{\psi} \end{aligned}$$

This gives us

$$\begin{aligned} \omega_1^2 + \omega_2^2 = \dot{\phi}^2 \sin^2\theta + \dot{\theta}^2, \qquad \omega_3^2 = (\dot{\phi}\cos\theta + \dot{\psi})^2 \\ \Rightarrow T = \frac{I_1}{2}\left(\dot{\phi}^2 \sin^2\theta + \dot{\theta}^2\right) + \frac{I_3}{2}(\dot{\phi}\cos\theta + \dot{\psi})^2 \end{aligned}$$

The potential energy is

$$V = -m_i \boldsymbol{r}_i \cdot \boldsymbol{g} = -M\boldsymbol{R} \cdot \boldsymbol{g} = Mgl\cos\theta$$

We can thus write down the Lagrangian,

$$L = T - V = \frac{I_1}{2}\left(\dot{\phi}^2 \sin^2\theta + \dot{\theta}^2\right) + \frac{I_3}{2}(\dot{\phi}\cos\theta + \dot{\psi})^2 - Mgl\cos\theta$$

It is seen that L is independent of ϕ which ψ; these are accordingly cyclic coordinates, and the corresponding generalized momenta p_ϕ, p_ψ are constant in time. This can also be seen by inspection: $\boldsymbol{N} = \boldsymbol{R} \times M\boldsymbol{g}$ are directed along the line of nodes, while z and z' both are orthogonal to the line of nodes. Thus $\boldsymbol{N}$ will have no component along z and z', meaning that there is no change of angular momentum about these these axes. The remaining generalized momenta are

$$\begin{aligned} p_\psi &= \frac{\partial L}{\partial \dot{\psi}} = I_3(\dot{\phi}\cos\theta + \dot{\psi}) = I_3\omega_3 = I_1 a = \text{time constant} \\ p_\phi &= \frac{\partial L}{\partial \dot{\phi}} = (I_1 \sin^2\theta + I_3 \cos^2\theta)\dot{\phi} + I_3\dot{\psi}\cos\theta = I_1 b = \text{time constant} \end{aligned}$$

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The constants a and b are defined above. In addition, the total energy is constant as the system is conservative:

$$E = V + T = \frac{I_1}{2}\left(\dot{\phi}^2 \sin^2\theta + \dot{\theta}^2\right) + \frac{I_3}{2}(\dot{\phi}\cos\theta + \dot{\psi})^2 + Mgl\cos\theta = \text{const.}$$

The equations for p_ϕ and p_ψ are now solved with respect to $I_3\dot{\psi}$ and combined. We get

$$I_1\dot{\phi}\sin^2\theta + I_1 a\cos\theta = I_1 b$$
$$\dot{\phi} = \frac{b - a\cos\theta}{\sin^2\theta}$$

which gives

$$\dot{\psi} = \frac{I_1 a}{I_3} - \cos\theta\frac{b - a\cos\theta}{\sin^2\theta}.$$

The kinetic energy in the rotating system becomes

$$E' \equiv E - \frac{I_3}{2}\omega_3^2 = \frac{I_1}{2}\dot{\theta}^2 + \frac{I_1}{2}\frac{(b - a\cos\theta)^2}{\sin^2\theta} + Mgl\cos\theta$$

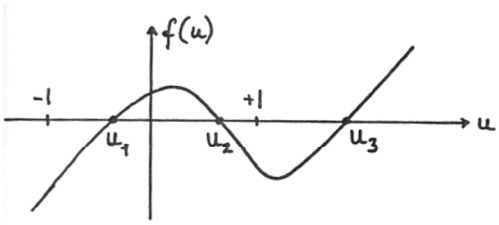
This expression is equivalent to a one-dimensional problem in the variable θ, with an effective potential

$$V'(\theta) = Mgl\cos\theta + \frac{I_1}{2}\frac{(b - a\cos\theta)^2}{\sin^2\theta}.$$

We substitute $u = \cos\theta$, and introduce new constants $\alpha = 2E'/I_1$ and $\beta = 2Mgl/I_1$. The equation for E' can then be rewritten, using $\sin^2\theta = 1 - \cos^2\theta$, to give

$$\begin{aligned}
E' &= \frac{I_1}{2}\frac{\dot{u}}{\sin^2\theta} + \frac{I_1}{2}\frac{(b - au)^2}{\sin^2\theta} + Mglu \\
\Longrightarrow E'(1 - u^2) &= \frac{I_1}{2}\dot{u}^2 + \frac{I_1}{2}(b - au)^2 + Mglu(1 - u^2) \\
\Longrightarrow \alpha(1 - u^2) &= \dot{u}^2 + (b - au)^2 + \beta u(1 - u^2) \\
\Longrightarrow \dot{u}^2 &= (1 - u^2)(\alpha - \beta u) - (b - au)^2 \\
&= \beta u^3 - (\alpha + a^2)u^2 + (2ab - \beta)u + \alpha - b^2 \equiv f(u)
\end{aligned}$$

The roots of the right-hand expression give $\dot{u} = 0$, i.e. $\dot{\theta} = -\dot{u}/\sin\theta = 0$. This gives the values of the angles for which $\dot{\theta}$ changes sign.



We have

$$f(\pm 1) = -(b \mp a)^2 < 0 \text{ and}$$
$$\lim_{u\to\pm\infty} f(u) = \pm\infty$$

which means that there exists at least one root $u_3 > 1$ which is nonphysical ($|u| = |\cos\theta| \leq 1$ when θ is real)! Physically acceptable values are obtained when $f(u) = \dot{u}^2 \geq 0$, i.e. u between u_1 and u_2 (which both have absolute values less than 1). Thus, θ can only take values such that $\cos\theta \in \langle u_1, u_2\rangle$. The motion can be illustrated by a curve which the z-axis draws on the surface of a unit sphere with center in the fixed point:

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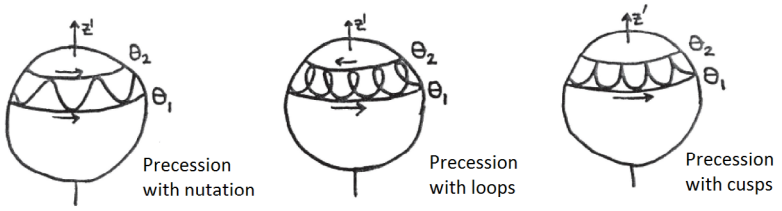
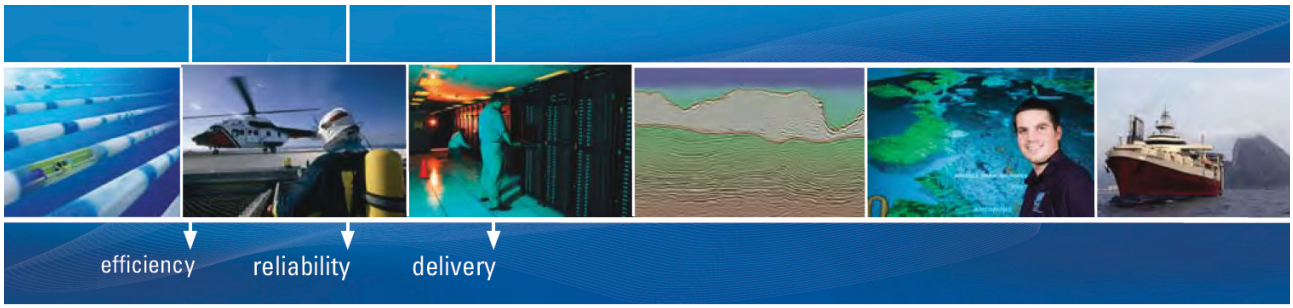


What is the condition for a *regular* precession to occur? The angle θ is then a constant, $\theta(t) = \theta(t = 0) \equiv \theta_0$. Moreover, $\theta_1 = \theta_2 = \theta_0$, so that $f(u)$ must have a double root. We get two equations, $f(u_0) = 0$ and $df(u_0)/du = 0$.
The first equation gives

$$\alpha - \beta u_0 = \frac{(b - au_0)^2}{1 - u_0^2}$$

and the second, $df(u_0)/du = 0$, gives

$$\frac{\beta}{2} = \frac{a(b - au_0)}{1 - u_0^2} - u_0 \frac{\alpha - \beta u_0}{1 - u_0^2}.$$



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Combining the two equations we get

$$\frac{\beta}{2} = \frac{a(b-au_0)}{1-u_0^2} - u_0\left(\frac{b-au_0}{1-u_0^2}\right)^2.$$

From above we have

$$\dot{\phi} = \frac{b-a\cos\theta_0}{\sin^2\theta_0} = \frac{b-au_0}{1-u_0^2},$$

so that

$$\frac{\beta}{2} = a\dot{\phi} - \dot{\phi}^2\cos\theta_0.$$

Inserting $\beta = Mgl/I_1$ and $a = I_3\omega_3/I_1 = I_3(\dot{\psi}+\dot{\phi}\cos\theta_0)/I_1$ we get

$$\begin{aligned} Mgl &= \dot{\phi}(I_3\omega_3 - I_1\dot{\phi}\cos\theta_0) \\ \Longrightarrow \dot{\phi} &= \frac{I_3\omega_3 \pm \sqrt{I_3^2\omega_3^2 - 4MglI_1\cos\theta_0}}{2I_1\cos\theta_0}. \end{aligned}$$

We require $\dot{\phi}$ to be real, so that the radicand has to be non-negative:

$$I_3^2\omega_3^2 \geq 4MglI_1\cos\theta_0.$$

From this we can conclude

- for $\theta_0 > \pi/2$, i.e. $\cos\theta_0 < 0$, a regular precession is possible for arbitrary values of ω_3,
- for $\theta_0 < \pi/2$, i.e. $\cos\theta_0 > 0$, a regular precession is possible only if $\omega_3 > \frac{2}{I_3}\sqrt{MglI_1\cos\theta_0}$.

The two roots of $\dot{\phi}$ are associated with "slow" and "fast" precession.

Let us go back to $Mgl = \dot{\phi}(I_3\omega_3 - I_1\dot{\phi}\cos\theta_0)$. With very slow precession one has $I_1\dot{\phi}\cos\theta_0 \ll I_3\omega_3$, i.e.

$$\dot{\phi} \approx \frac{Mgl}{I_3\omega_3}.$$

With *fast* precession the situation is reversed, as $Mgl \ll$ terms on the terms on the right hand side. In this case we get the root

$$\dot{\phi} \approx \frac{I_3\omega_3}{I_1\cos\theta_0}.$$

If $f(u=1)=0$, then $\theta = 0$ is a "bouncing angle". We shall consider this case more closely. Assume that $\theta = 0$ at $t = 0$. Then $p_\phi = p_\psi$, and therewith $a = b$ according to our definitions above.
We now obtain for E':

$$\begin{aligned} E' = E - \frac{I_3}{2}\omega_3^2 &= \frac{I_1}{2}\underbrace{\dot{\theta}^2}_{=0} + \frac{I_1 a}{2}\underbrace{\lim_{\theta\to 0}\frac{(1-\cos\theta)^2}{\sin^2\theta}}_{=0} + Mgl = Mgl \\ \Longrightarrow \alpha \equiv \frac{2E'}{I_1} &= \frac{2Mgl}{I_1} = \beta, \\ \Longrightarrow \dot{u}^2 &= (1-u^2)\beta(1-u) - a^2(1-u)^2 = (1-u)^2\left[\beta(1+u) - a^2\right], \end{aligned}$$

that means, $u = 1$ is a double root and we get $u_3 = a^2/\beta - 1$.

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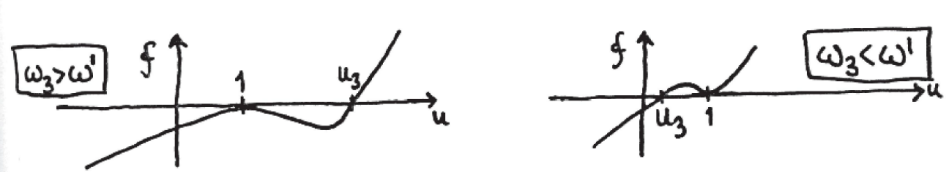
All together:

- $\frac{a^2}{\beta} > 2$ (fast precession) $\Longrightarrow u_3 > 1 \Longrightarrow$ only possible with $u = 1$, i.e. $\theta = 0$,
- $\frac{a^2}{\beta} < 2 \Longrightarrow u_3 < 1 \Longrightarrow$ nutation between $\theta = 0$ and $\theta = \theta_3$.



In the limiting case $a^2/\beta = 2$ we get

$$\frac{I_3^2 \omega'^2}{2MglI_1} = 2$$
$$\Longrightarrow \omega' = \frac{2}{I_3}\sqrt{MglI_1}$$

We thus see that the spinning top is not only a simple toy!

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VI. SMALL-SCALE, COUPLED OSCILLATIONS

Youtube-videos. 29-32 in this playlist.

Learning goals. After reading this chapter, the student should:

- Understand how a coupled system of oscillators can be mathematically analyzed
- Know how to compute the eigenfrequencies of a system
- Understand the concept of normal-coordinates and their relation to eigenfrequencies

A. Coupled oscillators

As a preliminary to the concepts that we will introduce in this chapter, let us briefly recap some of the main points for a 1D harmonic oscillator. It is described by $V(x) = kx^2/2$ so that the curvature is given by $\partial^2 V/\partial x^2 = k$. The resulting force is $F = m\ddot{x}$, giving rise to the equation of motion

$$m\ddot{x} + kx = 0. \tag{6.1}$$

The solution is $x(t) = \mathrm{Re}\{A\mathrm{e}^{-\mathrm{i}\omega_0 t}\}$ where $\omega_0 = \sqrt{k/m}$. This is a harmonic oscillation with frequency ω_0. We may include friction, corresponding to a damping which eventually terminates the oscillation, by adding a force proportional to the velocity of the particle: $F_f = -\lambda\dot{x}$. We obtain

$$m\ddot{x} + \lambda\dot{x} + kx = 0. \tag{6.2}$$

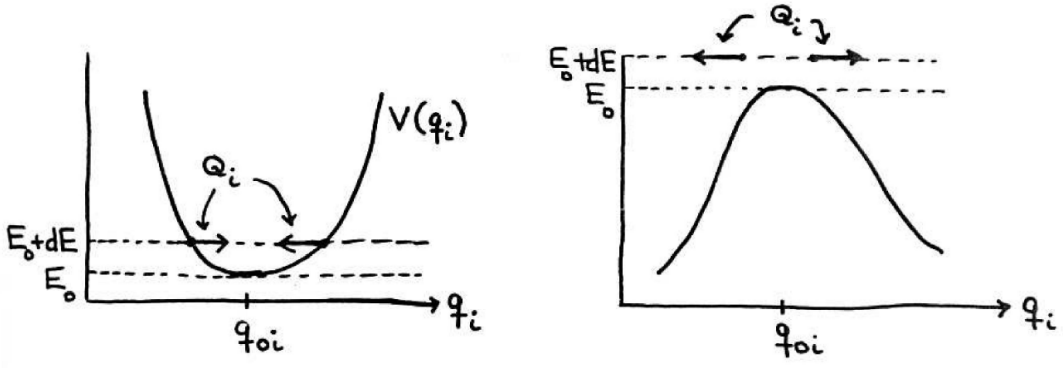
The solution reads $x(t) = \mathrm{e}^{-\lambda t/m}\mathrm{Re}\{A\mathrm{e}^{-\mathrm{i}\omega_0 t}\}$ which is then a damped harmonic oscillation. In the rest of this chapter, we will see how these concepts generalize from one single harmonic oscillator to a set of coupled harmonic oscillators.

Assume that that we have a conservative system, i.e. V only depends on position. Any constraints that are present are taken as time-independent. As usual, we may consider a general scenario with N "particles" and thus $3N$ degrees of freedom. With k constraints, the number of degrees of freedom is reduced to $n = 3N - k$. We may then describe the system via the n generalized and independent coordinates $(q_1, q_2, \ldots, q_n)$.

A system in equilibrium is obtained when all generalized forces vanish:

$$Q_i = -\left(\frac{\partial V}{\partial q_i}\right)_0 = 0. \tag{6.3}$$

In other words, V has an extremal value in the equilibrium configuration $(q_{0,1}, q_{0,2}, \ldots, q_{0,n})$. A *stable* equilibrium is characterized by the fact that a small perturbation from the equilibrium configuration only leads to a minor bound movement around this configuration. In contrast, *unstable* equilibrium is characterized by a small perturbation from the equilibrium configuration yielding unbound motion.



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We will here be concerned with small deviations from stable equilibrium, thus giving rise to a bound movement. We write $q_i = q_{0,i} + \eta_i$ where η_i represents the deviation from the equilibrium position $q_{0,i}$. Since $\{q_{0,i}\}$ are constants, we may choose η_i as new generalized coordinates. It is useful to Taylor-expand V around $q_{0,i}$ which provides:

$$V(q_1, q_2, \ldots, q_n) = V(q_{0,1}, q_{0,2}, \ldots, q_{0,n}) + \Big(\frac{\partial V}{\partial q_i}\Big)_0 \eta_i + \frac{1}{2}\Big(\frac{\partial^2 V}{\partial q_i \partial q_j}\Big)_0 \eta_i \eta_j + \ldots \tag{6.4}$$

Note that we are using the summation convention with repeated indices. The first order derivative vanishes due to $(\partial V/\partial q_i)_0 = 0$ in equilibrium, as stated above. We also have the freedom of choosing our reference level for energy as we please, so might as well set $V(q_{0,1}, q_{0,2}, \ldots, q_{0,n}) = 0$. This means that our zero-energy level is the equilibrium configuration. We are left with:

$$V = \frac{1}{2}\Big(\frac{\partial^2 V}{\partial q_i \partial q_j}\Big)_0 \eta_i \eta_j \equiv \frac{1}{2} V_{ij} \eta_i \eta_j. \tag{6.5}$$

It follows that we may set $V_{ij} = V_{ji}$.

The kinetic part of the energy can be written more generally by making it a quadratic function of the velocities:

$$T = \frac{1}{2} m_{ij} \dot{q}_i \dot{q}_j = \frac{1}{2} m_{ij} \dot{\eta}_i \dot{\eta}_j. \tag{6.6}$$

Note that the coefficients m_{ij} can depend on the coordinates q_k:

$$m_{ij}(q_1, q_2, \ldots, q_n) = m_{ij}(q_{0,1}, q_{0,2}, \ldots) + \Big(\frac{\partial m_{ij}}{\partial q_k}\Big)_0 \eta_k + \ldots \tag{6.7}$$

For instance, if we write the kinetic energy T in polar coordinates, we know that $T = m\dot{r}^2/2 + mr^2\dot{\theta}^2/2$. Comparison with the above allows us to identify $m_{11} = m, m_{22} = mr^2, m_{12} = m_{21} = 0$. Now, since we're interested in small deviations η_i from equilibrium, we only keep terms up to second order of η_i in T:

$$T = \frac{1}{2} T_{ij} \dot{\eta}_i \dot{\eta}_j \text{ where } T_{ij} = m_{ij}(q_{0,1}, q_{0,2}, \ldots) \tag{6.8}$$

Often, T_{ij} will be diagonal: $T_{ij} = T_i \delta_{ij}$.

We are now in a position to write down the total Lagrange function:

$$L(\eta, \dot{\eta}) = T - V = \frac{1}{2}(T_{ij} \dot{\eta}_i \dot{\eta}_j - V_{ij} \eta_i \eta_j). \tag{6.9}$$

Using Lagrange's equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\eta}_i} - \frac{\partial L}{\partial \eta_i} = 0, \; i = 1, 2, \ldots n \tag{6.10}$$

we obtain the equations of motion determining the time-evolution of the deviations η_i:

$$T_{ij} \ddot{\eta}_j + V_{ij} \eta_j = 0 \tag{6.11}$$

This is a set of n coupled 2nd order differential equations. The solution of this equation η_j describes the motion of the system near equilibrium.

We now look for solutions of this equation in the form of oscillations:

$$\eta_i(t) = A_i \mathrm{e}^{-\mathrm{i}\omega t}. \tag{6.12}$$

Here, A_i are complex amplitudes. However, it is implicitly understood that it is $\mathrm{Re}\{\eta_i\}$ that corresponds to the real physical motion. We only work with complex quantities because it is mathematically more convenient than working with $\cos$ and $\sin$. Inserting this *ansatz* into the equation of motion, we get

$$V_{ij} A_j = \omega^2 T_{ij} A_j = 0. \tag{6.13}$$

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These are now n homogeneous equations for the amplitudes A_j. From the theory of linear algebra, we know that such a system has a non-trivial solution for A_j if the following condition is satisfied:

$$\det(\hat{V} - \omega^2 \hat{T}) = 0 \tag{6.14}$$

where $\hat{V}$ is the potential energy matrix with entries $\hat{V}_{ij} = V_{ij}$ and similarly for $\hat{T}$. This equation determines the allowed *eigenfrequencies* of the system ω. There may be as many as n different eigenfrequencies: however, there could also be degenerate values for ω. Let us denote the eigenfrequencies $\{\omega_\alpha\}$. Physically, we must demand that ω_α are all real numbres. If not, we could write $\omega_\alpha = \omega' + \mathrm{i}\omega''$, giving us a solution $\eta_i \propto \eta\omega'' t$. This would be either exponential increas ($\omega'' > 0$) or damping ($\omega'' < 0$) of the motion, which is not consistent with energy conservation.

By solving Eq. (6.14), one finds ω_α. The next question is then: what do the corresponding amplitudes look like? Which parts of the system are moving, and how much are they moving, when they are oscillating in the mode α? To answer this question, we must determine the amplitudes $A_{i\alpha}$: the amplitude of the oscillation along generalized coordinates q_i in the mode α. The amplitude is, according to the above, determined by the equations

$$(V_{ij} - \omega_\alpha^2 T_{ij}) A_{j\alpha} = 0. \tag{6.15}$$

For a given ω_α, this are n equations determining $n - 1$ of the components in the amplitude vector:

$$\boldsymbol{A}_\alpha = \begin{pmatrix} A_{1\alpha} \\ A_{2\alpha} \\ \dots A_{n\alpha} \end{pmatrix} \tag{6.16}$$

We are left with one undetermined component for every α, for instance $A_{1\alpha}$. Since $A_{1\alpha}$ is in general complex, there are 2 undetermined coefficients (the real and imaginary part or, equivalently, the amplitude and phase of $A_{1\alpha}$) for each α. This is the case for each generalized coordinate, so in total we have $2n$ undetermined quantities. This is in agreement with the fact that we need $2n$ initial conditions to solve Lagranges equations and determine the solutions completely.

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Let us to begin with treat the case where all eigenfrequences ω_α are different. Our task is then to show that $A_{i\alpha}$ is proportional to the *minor* $\Delta_{i\alpha}$ of the determinant $|\hat{V} - \omega_\alpha^2 \hat{T}|$. The minor (also known as cofactor) $\Delta_{i\alpha}$ is defined as the subdeterminant that one obtains by removing row i and column α from the original determinant. The sign of $\Delta_{i\alpha}$ is given by $(-1)^{i+\alpha}$. Rather than giving a general proof that $A_{i\alpha} \propto \Delta_{i\alpha}$, we show it for a specific case in order to make the notation less overwhelming. Consider the case with $n = 3$ and the equation for $\alpha = i = 1$:

$$\sum_{j=1}^{n} (V_{ij} - \omega_\alpha^2 T_{ij}) A_{j\alpha} = 0. \tag{6.17}$$

We write this out as

$$(V_{11} - \omega_1^2 T_{11}) A_{11} + (V_{21} - \omega_1^2 T_{21}) A_{21} + (V_{31} - \omega_1^2 T_{31}) A_{31} = 0. \tag{6.18}$$

Now compare this expression with the equation we obtain from $|\hat{V} - \omega_\alpha^2 \hat{T}| = 0$ by setting $\alpha = 1$ and expanding the determinant along the 1st column:

$$(V_{11} - \omega_1^2 T_{11}) \Delta_{11} + (V_{21} - \omega_1^2 T_{12}) \Delta_{21} + (V_{31} - \omega_1^2 T_{31}) \Delta_{31} = 0 \tag{6.19}$$

Since $\hat{V}$ and $\hat{T}$ both are symmetric, we may exchange the indices i and j in the equations with the A's. By afterwards writing $A_{i\alpha} = C_\alpha \Delta_{i\alpha}$ where C_α is a complex constant of proportionality, we arrive at

$$C_1[(V_{11} - \omega_1^2 T_{11}) \Delta_{11} + (V_{21} - \omega_1^2 T_{12}) \Delta_{21} + (V_{31} - \omega_1^2 T_{31}) \Delta_{31}] = 0 \tag{6.20}$$

which is precisely the characteristic equation, obtained by using $A_{i\alpha} \propto C_\alpha$.

We may now write the solution for $\eta_{i\alpha}$ as follows:

$$\eta_{i\alpha} = C_\alpha \Delta_{i\alpha} \mathrm{e}^{-\mathrm{i}\omega_\alpha t}, \tag{6.21}$$

so that the general solution for the real motion of the generalized coordinate η_i becomes:

$$\mathrm{Re}\eta_i(t) = \mathrm{Re} \sum_{\alpha=1}^{n} \eta_{i\alpha}(t) = \mathrm{Re} \sum_{\alpha=1}^{n} C_\alpha \Delta_{i\alpha} \mathrm{e}^{-\mathrm{i}\omega_\alpha t}. \tag{6.22}$$

The time variation of η_i is thus a superposition of n harmonic oscillations with phases and amplitudes determined by the initial conditions and frequencies fixed by the potential and kinetic energy matrices of the system $\hat{V}$ and $\hat{T}$. It is convenient to here introduce new independent coordinates Θ_α according to

$$\Theta_\alpha(t) = \mathrm{Re}\{C_\alpha \mathrm{e}^{-\mathrm{i}\omega_\alpha t}\}, \tag{6.23}$$

so that the solution is

$$\mathrm{Re}\eta_i(t) = \sum_{\alpha=1}^{n} \Delta_{i\alpha} \Theta_\alpha(t). \tag{6.24}$$

We will now show that the equations of motion for $\Theta_\alpha(t)$ are *uncoupled*:

$$\ddot{\Theta}_\alpha + \omega_\alpha^2 \Theta_\alpha = 0, \ \alpha = 1, 2, \ldots \tag{6.25}$$

We will refer to Θ_α as the normal-coordinates. The system oscillates in normalmode α with eigenfrequency ω_α. To see this, let us insert the normalmodes into our expressions for kinetic and potential energy:

$$\begin{aligned} T &= \frac{1}{2} T_{ij} \mathrm{Re}\dot{\eta}_i \mathrm{Re}\dot{\eta}_j = \frac{1}{2} T_{ij} \Delta_{i\alpha} \dot{\Theta}_\alpha \Delta_{j\beta} \dot{\Theta}_\beta, \\ V &= \frac{1}{2} V_{ij} \mathrm{Re}\eta_i \mathrm{Re}\eta_j = \frac{1}{2} V_{ij} \Delta_{i\alpha} \Theta_\alpha \Delta_{j\beta} \Theta_\beta. \end{aligned} \tag{6.26}$$

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Note that we must take the real part of η_i and η_j before multiplying instead of *after* multiplying, since it is Re$\{\eta_i\}$ that corresponds to the true physical motion (taking the real part after multiplication would give a spurious contribution from the product of the imaginary parts of η_i and η_j). The expression for V can be rewritten by using that:

$$V_{ij}A_{j\alpha} = \omega_\alpha^2 T_{ij}A_{j\alpha} \rightarrow V_{ij}\Delta_{j\alpha} = \omega_\alpha^2 T_{ij}\Delta_{j\alpha}. \tag{6.27}$$

Now, we wish to see if we can manipulate the factor $\sum_{i,j=1}^{n} T_{ij}\Delta_{i\alpha}\Delta_{j\beta}$ somehow, since it appears both in the expression for T and V. We have noted previously that the following equation is satisfied:

$$\sum_{j=1}^{n}(V_{ij} - \omega_\alpha^2 T_{ij})A_{j\alpha} = 0. \tag{6.28}$$

Let us write this equation both for α and β:

$$\begin{aligned}\sum_j V_{ij}\Delta_{j\alpha} &= \omega_\alpha^2 \sum_j T_{ij}\Delta_{j\alpha},\\ \sum_j V_{ij}\Delta_{j\beta} &= \omega_\beta^2 \sum_j T_{ij}\Delta_{j\beta}.\end{aligned} \tag{6.29}$$

By using $A_{j\alpha} = C_\alpha\Delta_{j\alpha}$ and multiplying the lower line of Eq. (6.29) with $\sum_i \Delta_{i\alpha}$, we get

$$\sum_{ij}\Delta_{i\alpha}V_{ij}\Delta_{j\beta} = \sum_{ij}\Delta_{i\alpha}\omega_\beta^2 T_{ij}\Delta_{j\beta}. \tag{6.30}$$

By using that $V_{ij} = V_{ji}$ and similarly for T, Eqs. (6.29) and (6.30) can now be combined into

$$(\omega_\alpha^2 - \omega_\beta^2)\sum_{ij} T_{ij}\Delta_{i\alpha}\Delta_{i\beta} = 0. \tag{6.31}$$

It is clear that if $\omega_\alpha \neq \omega_\beta$, it is the sum that has to be zero. However, if $\alpha = \beta$, then the sum does not have to be zero.

From our definition of $\Delta_{i\alpha}$ as the minor (i,α) of the determinant $|\hat{V} - \omega_\alpha^2\hat{T}|$, we are not allowed to *choose* one particular value for $\sum_{ij} T_{ij}\Delta_{i\alpha}\Delta_{j\alpha}$ since both Δ's are uniquely defined. However, let us modify our previous statement slightly and instead say that $\Delta_{i\alpha}$ is proportional to the minor. This is justified as follows. We showed previously that $A_{i\alpha}$ is proportional to the minor via a complex coefficient C_α. Thus, it should work equally well to set

$$A_{i\alpha} = C'_\alpha\Delta_{i\alpha} \tag{6.32}$$

with new coefficients of proportionality C'_α and then saying that $\Delta_{i\alpha}$ is just proportional to the minor. So what is the gain in doing this? The point is we now have the freedom to choose a specific value for $\sum_{ij} T_{ij}\Delta_{i\alpha}\Delta_{j\alpha}$. In other words, we can *choose* the normalization of $\Delta_{i\alpha}$. A particularly convenient choice is to choose:

$$\sum_{ij} T_{ij}\Delta_{i\alpha}\Delta_{j\beta} = \delta_{\alpha\beta}. \tag{6.33}$$

The purpose of this choice for normalization is that we can now simplify the expressions for T and V expressed in terms of the normal-coordinates. We obtain:

$$\begin{aligned}T &= \frac{1}{2}\sum_{\alpha\beta}\sum_{ij} T_{ij}\Delta_{i\alpha}\Delta_{j\beta}\dot{\Theta}_\alpha\dot{\Theta}_\beta = \frac{1}{2}\sum_\alpha(\dot{\Theta}_\alpha)^2,\\ V &= \frac{1}{2}\sum_{\alpha\beta}\sum_{ij} T_{ij}\Delta_{i\alpha}\Delta_{j\beta}\omega_\beta^2\Theta_\alpha\Theta_\beta = \frac{1}{2}\sum_\alpha \omega_\alpha^2\Theta_\alpha^2.\end{aligned} \tag{6.34}$$

The Lagrange function $L = T - V$ then becomes, expressed in terms of the normal-coordinates as independent variables,

$$L = \frac{1}{2}\sum_\alpha[(\dot{\Theta}_\alpha^2)^2 - \omega_\alpha^2\Theta_\alpha^2] \tag{6.35}$$

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Lagrange's equations $(d/dt)(\partial L/\partial \dot{\Theta}_\alpha) - \partial L/\partial \Theta_\alpha = 0$ then take the form:

$$\ddot{\Theta}_\alpha + \omega_\alpha^2 \Theta_\alpha = 0. \tag{6.36}$$

This is a remarkable result: the equations are now completely decoupled and can be solved once the eigenfrequencies ω_α have been determined and by using appropriate boundary conditions. Note that if two or more of the eigenfrequencies ω_α are degenerate, the procedure becomes slightly modified.

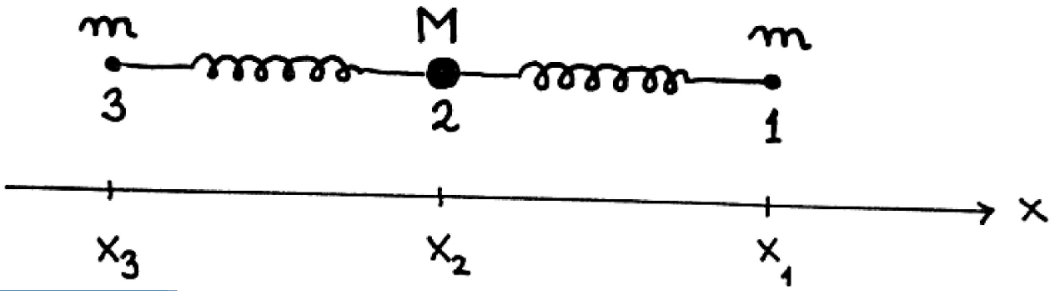
B. Application to a triatomic linear symmetric molecule (CO_2)

Consider the CO_2 molecule where the atoms are linearly arranged (O=C=O), see figure below. In equilibrium, the distance between the atoms is written as

$$x_{01} - x_{02} = x_{02} - x_{03} = b. \tag{6.37}$$

The deviation from equilibrium can thus be written as

$$\eta_i = x_i - x_{0i},\ i = 1, 2, 3. \tag{6.38}$$



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Assume that only the nearest neighbors are interacting via a harmonic potential:

$$V = \frac{1}{2}k[(x_1 - x_2) - b]^2 + \frac{1}{2}k[(x_2 - x_3) - b]^2 = (k/2)(\eta_1 - \eta_2)^2 + (k/2)(\eta_2 - \eta_3)^2. \tag{6.39}$$

The kinetic energy is

$$T = (m/2)\dot{x}_1^2 + (m/2)\dot{x}_3^2 + (M/2)\dot{x}_2^2 = (m/2)(\dot{\eta}_1^2 + \dot{\eta}_3^2) + (M/2)\dot{\eta}_2^2. \tag{6.40}$$

The Lagrange function is $L = T - V$ as usual. We can simplify the situation by assuming that the center of mass is at rest, which still allows for the possibilities of vibrations of the atoms relative each other. The center of mass position thus satisfies:

$$m(\eta_1 + \eta_3) + M\eta_2 = 0. \tag{6.41}$$

Let us define the new coordinates

$$Q_a = \eta_1 + \eta_3,\ Q_s = \eta_1 - \eta_3. \tag{6.42}$$

It will later transpire why the subscripts 'a' and 's' are suitable for these coordinates. In terms of the new coordinates, we obtain:

$$\eta_1 = (Q_a + Q_s)/2,\ \eta_3 = (Q_a - Q_s)/2,\ \eta_2 = -mQ_a/M. \tag{6.43}$$

by using the fact that the center of mass is at rest. By expressing L in terms of Q_a and Q_s instead of the η_i quantities, we get after some algebra:

$$L = \frac{m}{4}\frac{\mu}{M}\dot{Q}_a^2 + \frac{m}{4}\dot{Q}_s^2 - \frac{k}{2}\Big[2\Big(\frac{\mu}{2M}\Big)^2 Q_a^2 + Q_s^2/2\Big] \tag{6.44}$$

We introduced the total mass $\mu = M + 2m$. An important observation is that *there are no cross-terms between Q_a and Q_s in the above expression*. This means that Q_a and Q_s are in fact the normal coordinates of the system: their corresponding Lagrange equations are decoupled. In fact, we can immediately identify the eigenfrequencies by first introducing the rescaled quantities

$$\Theta_s = \sqrt{m/2}\,Q_s,\ \Theta_a = \sqrt{m\mu/(2M)}\,Q_a \tag{6.45}$$

which gives

$$L = \frac{1}{2}[\dot{\Theta}_s^2 - \frac{k}{m}\Theta_s^2 + \dot{\Theta}_a^2 - \frac{k\mu}{mM}\Theta_a^2]. \tag{6.46}$$

Based on the general form of the Lagrange equations for normal-coordinates derived previously, we see that the eigenfrequencies are:

$$\omega_s = \sqrt{k/m},\ \omega_a = \sqrt{k\mu/(mM)}. \tag{6.47}$$

Now, we did "cheat" a little bit by introducing the normal-coordinates right away - under usual circumstances, it could be difficult to just guess which linear combination of the original coordinates that provide the normal-coordinates of the system. However, an important clue was that all cross-terms between Q_a and Q_s were removed. Thus, one viable strategy would be to look for a coordinate transformation which removes all cross-terms in the Lagrange function: the new coordinates obtained in this way should be the normal-coordinates.

If we didn't know this, we could still find the eigenfrequencies simply by computing the determinant $|\hat{V} - \omega^2\hat{T}| = 0$. The elements of V_{ij} and T_{ij} are determined from the general form

$$T = \frac{1}{2}\sum_{ij} T_{ij}\dot{\eta}_i\dot{\eta}_j,\ V = \frac{1}{2}\sum_{ij} V_{ij}\eta_i\eta_j. \tag{6.48}$$

Comparing with our expressions for T and V for the present triatomic molecule, one finds

$$\hat{V} = \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix},\ \hat{T} = \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix}. \tag{6.49}$$

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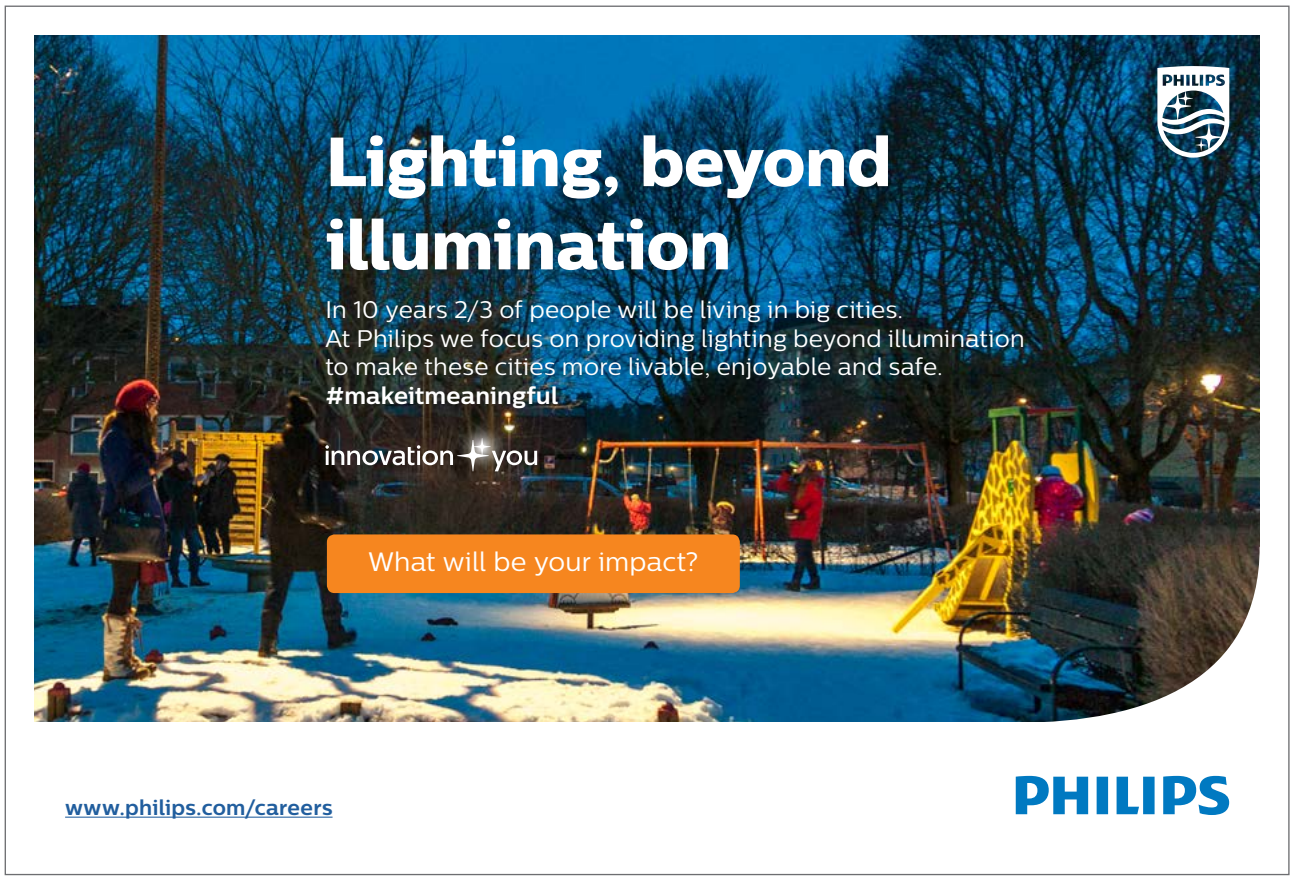
Evaluating the determinant gives the following result:

$$\omega^2(k - \omega^2 m)(k\mu - \omega^2 mM) = 0. \tag{6.50}$$

This equation has three solutions:

$$\begin{aligned} \omega_1 &= 0, \\ \omega_2 &= \omega_s, \\ \omega_3 &= \omega_a. \end{aligned} \tag{6.51}$$

Hang on - when we introduced the normal-coordinates, we found only two eigenfrequencies. Why are there three now? Before continuing to read, take a moment to consider this question. Is there some difference in the assumptions we made when using the normal-coordinate method and the calculation of the determinant? The answer is yes: when expressing the Lagrange function with the normal-coordinates we made the simplifying assumption that the center of mass was at rest. In contrast, we did not make that assumption when finding the eigenfrequencies from the determinant and hence we found one more solution: $\omega = 0$, which corresponds precisely to uniform translational motion of the entire molecule (no relative motion between the atoms)! The two other solutions ω_2 and ω_3 are the same ones as we found before. Now, $\omega_2 = \omega_s$ is the so-called symmetric mode which corresponds to the two oxygen atoms oscillating in phase toward the carbon atom (thus moving in opposite directions at all times) whereas $\omega_3 = \omega_a$ is the antisymmetric mode where the two oxygen atoms move in the same direction while the carbon atom moves in the opposite direction of the oxygen. Note that in both cases, the center of mass is at rest.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VII. THE THEORY OF SPECIAL RELATIVITY

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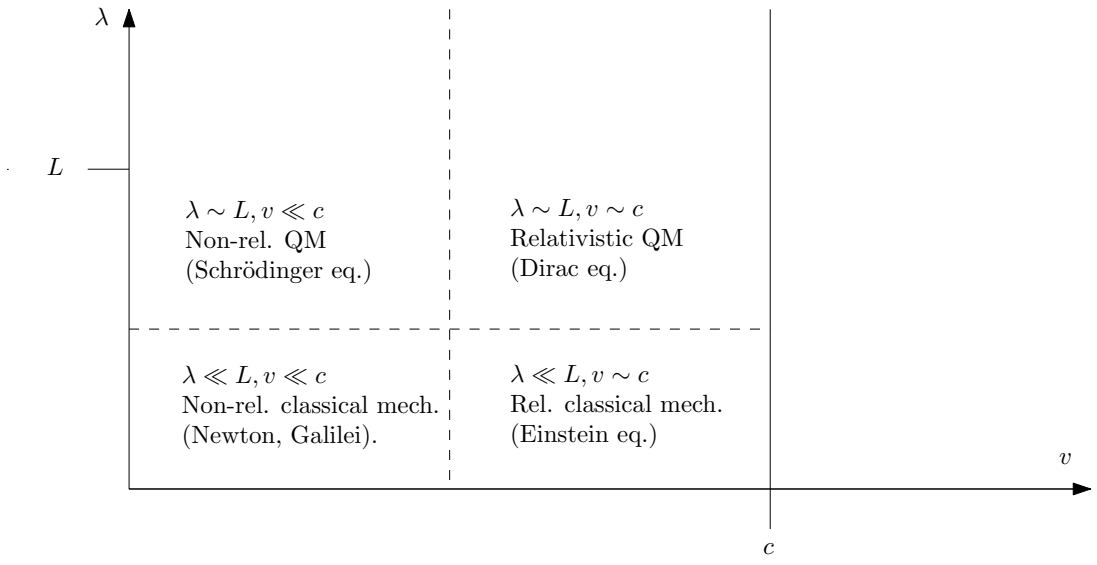
Learning goals. After reading this chapter, the student should:

- Understand the concepts of Lorentz-transformations, Lorentz-invariance, and Minkowski-space
- Be familiar with 4-vectors and their mathematical properties
- Be able to solve elementary problems in relativistic mechanics, such as scattering of particles
- Be able to explain the concept of threshold energy and know about how EM fields transform relativistically

A. Introductory remarks

Assume that we are considering a system which size is characterized by a length L. Let $\lambda = h/p$ be the de Broglie wavelength for a body in the system moving with momentum p (h is Planck's constant). Finally, v is a typical velocity for a body in the system while c is the speed of light. With these definitions, we can now characterize the realm of physics with four quadrants as depicted in the below figure.



In this chapter, we will consider systems in the lower right quadrant where the typical size of the system far exceeds the de Broglie wavelength of particles in it, but where the velocities under consideration are comparable to the speed of light. This is the realm of Einstein's special theory of relativity. For accelerated inertial frames and for a more thorough treatment of gravitation in relativistic physics, one must turn to Einstein's general theory of relativity. Although of interest, we will here not focus on early experiments (Michelson-Morley), philsophical perspectives on relativity, and apparent paradoxes. Instead, our goal is to use the formalism and toolbox that we have developed so far in classical mechanics to describe the special theory of relativity.

A concept we will frequently draw upon is that of an inertial frame. The definition of such a frame is that Newton's law is valid: objects will move in a straight line with constant velocity unless acted upon by some force. This is *e.g.* not the case in accelerated frames, where there exists fictious forces such as the Coriolis force. All inertial frames are thus in a state of constant, linear motion relative each other. In order to swap between the coordinates of two inertial frames S and S', where S' is moving with velocity $\boldsymbol{v}$ relative S, you might be accustomed to using the Galilei transformation:

$$\boldsymbol{r}' = \boldsymbol{r} - \boldsymbol{v}t, t' = t. \tag{7.1}$$

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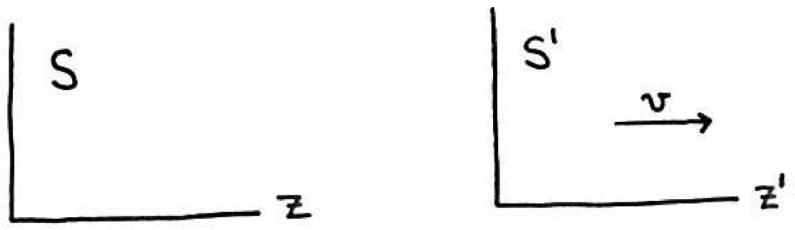
There is a problem with this transformation. It predicts that the speed of light should be different in S' and S: $c' = c - v$. However, it is experimentally known that the speed of light is the same in S' and S, $c' = c$, thus independent on the relative velocity between the inertial frames. The two basic postulates of Einstein's theory of special relativity are:

- The laws of physics are the same in all inertial frames. This is called the principle of relativity, which is also satisfied in Newtonian mechanics.
- The speed of light in vacuum has the same constant value in all inertial frames and is independent on the motion of the light-source.

B. Lorentz transformations

Two inertial frames S and S' are shown in the figure. S' is moving with a velocity $\boldsymbol{v}$ relative S. Assume that their origos coincide at $t = t' = 0$ and that $\boldsymbol{v} \parallel \hat{z}$. The Lorentz-transformation is then defined as follows:

$$x' = x,\ y' = y,\ z' = \gamma(z - vt),\ t' = \gamma(t - vz/c^2),$$
$$\gamma = 1/\sqrt{1-\beta^2},\ \beta = v/c. \tag{7.2}$$



The inverse transformation is obtained by $v \to -v$. Note that the transformation equations are linear. The Lorentz-transformation is designed specifically to make the speed of light c invariant, i.e. the same seen from both systems S and S'. Let us prove this important result explicitly.

Assume that there is a source in the origo of S' that emits a light-wave at $t = 0$. The equation for the light-wave is then:

$$r' = ct' \to (x')^2 + (y')^2 + (z')^2 = c^2(t')^2. \tag{7.3}$$

If we now express (x', y', z', t') with (x, y, z, t) via Eq. (7.2) and insert the resulting expression in Eq. (7.3), one obtains

$$x^2 + y^2 + z^2 = c^2t^2. \tag{7.4}$$

In effect, the equation for the light-wave in S is identical to that in S'. We see that the light-wave moves with velocity c both in S and S'. Note that in the non-relativistic limit $v \ll c$, the Lorentz-transformation Eq. (7.2) reduces to the Galilei transformation. For an arbitrary relative velocity vector $\boldsymbol{v}$ between S and S', the transformation becomes:

$$\boldsymbol{r}' = \boldsymbol{r} + (\gamma - 1)\frac{(\boldsymbol{\beta}\cdot\boldsymbol{r})\boldsymbol{\beta}}{\beta^2} - \gamma ct\boldsymbol{\beta},$$
$$t' = \gamma t - \frac{\gamma}{c}\boldsymbol{\beta}\cdot\boldsymbol{r}. \tag{7.5}$$

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where $\boldsymbol{\beta} = \boldsymbol{v}/c$.

Due to the fact that the Lorentz-transformation is linear, we can use the same framework as previously done for rotations. We introduce a "fourth dimension" via the variable $x_4 = \mathrm{i}ct$ so that the 4-dimensional Minkowski-space has axes

$$x_1 = x,\ x_2 = y,\ x_3 = z,\ x_4 = \mathrm{i}ct. \tag{7.6}$$

We see that

$$x^2 + y^2 + z^2 - c^2t^2 = x_1^2 + x_2^2 + x_3^2 + x_4^2 = \sum_{\mu=1}^{4} x_\mu x_\mu \equiv x_\mu x_\mu \tag{7.7}$$

where we used the sum convention for repeated indices. A vector in Minkowski-space is known as a 4-vector and describes an *event* taking place at a given position in time and space. To distinguish more clearly between 4-vectors and conventional 3-vectors, we will use Greek indices for 4-vectors $(\alpha, \beta, \mu, \ldots)$ and Roman indices for 3-vectors $(i, j, k, \ldots)$. The invariance of the speed of light can now be expressed by stating that $x_\mu x_\mu$ is invariant: it has the same value in all inertial frames. In other words, the norm of the "position vector" x_μ in Minkowski-space remains invariant under a Lorentz-transformation. The Lorentz-transformation is an orthogonal transformation in Minkowsi-space since it does not alter the norm of the 4-vector. This is in complete analogy to rotations in usual 3D space which also are orthogonal transformations since they do not change the length of a 3-vector.

We can also write the Lorentz-transformation in matrix form:

$$\mathbb{X}' = \hat{L}\mathbb{X} \text{ or } x'_\mu = L_{\mu\nu}x_\nu, \tag{7.8}$$

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where $\mathbb{X}$ denotes a 4-vector, i.e. $\mathbb{X} = (x, y, z, \mathrm{i}ct)$. Choosing the relative velocity along the z-axis gives the matrix:

$$\hat{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \gamma & \mathrm{i}\beta\gamma \\ 0 & 0 & -\mathrm{i}\beta\gamma & \gamma \end{pmatrix}. \tag{7.9}$$

For a velocity $\boldsymbol{v}$ in arbitrary direction ($\boldsymbol{\beta} = \boldsymbol{v}/c$), one has

$$L_{jk} = \delta_{jk} + (\gamma - 1)\beta_j\beta_k/\beta^2,\ L_{j4} = \mathrm{i}\gamma\beta_j,\ L_{4k} = -\mathrm{i}\gamma\beta_k,\ L_{44} = \gamma. \tag{7.10}$$

From our previous treatment of linear transformations, we know that an orthogonal matrix has the property $\hat{L}^{-1} = \hat{L}^{\mathrm{T}}$ where $^{\mathrm{T}}$ is the matrix transpose. The inverse Lorentz-transformation can thus be written

$$x_\mu = (\hat{L}^{-1})_{\mu\nu}x'_\nu = (\hat{L}^{\mathrm{T}})_{\mu\nu}x'_\nu = L_{\nu\mu}x'_\nu. \tag{7.11}$$

Sometimes, it is convenient to represent Lorentz-transformations as rotations with a complex angle. To see how this works, recall that the matrix

$$\begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \tag{7.12}$$

represents rotation with an angle ϕ in the two-dimensional plane. Thus, the Lorentz-transformation in Eq. (7.9) is equivalent to a rotation in the $x_3 - x_4$ plane with a complex angle ϕ determined by

$$\gamma = \cos\phi,\ \mathrm{i}\beta\gamma = \sin\phi. \tag{7.13}$$

When is this useful? It comes in handy when performign multiple successive transformations. Consider for instance a scenario where there are three inertial frames. S' is moving with velocity v relative S and S" is moving with velocity v' relative S'. The goal is to find the velocity with which system S" moves relative S. We know that $\mathbb{X}' = \hat{L}\mathbb{X}$ and $\mathbb{X}'' = \hat{L}'\mathbb{X}'$. Thus, we may write $\mathbb{X}'' = \hat{L}''\mathbb{X}$ if $\hat{L}'' = \hat{L}'\hat{L}$. The point is then that the "rotation" ϕ'' in Minkowsi-space taking us from S to S" must be equal to the total angle of rotation $\phi + \phi'$ in going from S to S' to S". Thus, we have $\phi'' = \phi' + \phi$. We obtain

$$\tan\phi'' = \frac{\sin\phi''}{\cos\phi''} = \mathrm{i}\beta''. \tag{7.14}$$

But we also have that:

$$\tan\phi'' = \tan(\phi' + \phi) = \frac{\sin(\phi' + \phi)}{\cos(\phi' + \phi)} = \frac{\tan\phi' + \tan\phi}{1 - \tan\phi\tan\phi'}. \tag{7.15}$$

Combining the two equations yields:

$$\mathrm{i}\beta'' = \mathrm{i}\frac{\beta' + \beta}{1 + \beta\beta'} \rightarrow v'' = \frac{v' + v}{1 + vv'/c^2}. \tag{7.16}$$

This is Einstein's addition formula. We see that $v'' \neq v' + v$, which would have been the non-relativistic result, and also $v'' < c$ even if $v \simeq c$ and $v' \simeq c$.

The properties of the Lorentz-matrix can be used to classify it further. Since it is orthogonal, we know that $|\hat{L}| = \pm 1$. If the determinant is equal to +1, we say that it is a *proper* Lorentz-transformation, meaning that it is possible to continuously transform it into the identity matrix $\hat{1}$ (if also $L_{44} \geq 1$). If the determinant is -1, it is an *improper* Lorentz-transformation. This is *e.g.* obtained by inverting the space-axes, but not the time-axis. If both the space- and time-axes are inverted, we have $\hat{L} = \mathrm{diag}(-1, -1, -1, -1)$ and thus $|\hat{L}| = +1$.

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C. Choices of metric

We here discuss some details about the choice of so-called *metric*. Let us first introduce the following concepts:

- **Riemann-space**: characterized by coordinates x_μ (which can be real or complex). An infinitesimal path element in this space has the square $ds^2 = g_{\mu\nu}dx_\mu dx_\nu$.
- **Metric tensor**: denoted $\hat{g}$ with matrix elements $g_{\mu\nu}$.

Covariant vector components have a lower index (x_μ) where as contravariant vector components have index up (x^μ). One trick to remember this is the following: "co is low"'. The metric tensor itself has the property $g_{\mu\nu} = g^{\mu\nu}$ and its effect is to raise and lower indices. For instance, one has

$$x_\mu = g_{\mu\nu}x^\nu,\ x^\mu = g^{\mu\nu}x_\nu. \tag{7.17}$$

For the infinitesimal path element, we may then write

$$ds^2 = dx_\mu dx^\mu. \tag{7.18}$$

For complex Minkowsi-space, we had $x_4 = \mathrm{i}ct$. Using $\hat{g} = \mathrm{diag}(1,1,1,1)$ gives us $ds^2 = dx^2 + dy^2 + dz^2 - c^2dt^2$ which we have seen is invariant (its value is the same in any inertial frame). For this choice of metric tensor $\hat{g}$, we see that $x_\mu = x^\mu$ and there is no distinction between covariant and contravariant vectors. This is a handy choice, but it comes at the expense of working with a complex variable x_4. This choice of metric is characterized by the fact that $\mathrm{Tr}\hat{g} = 4$. To see which alternatives we have, we could instead use

$$x^0 = ct, x^1 = x, x^2 = y, x^3 = z. \tag{7.19}$$

To keep $ds^2 = dx_\mu dx^\mu$ invariant, we then need to choose either $\hat{g} = \mathrm{diag}(-1,1,1,1)$ (which has $\mathrm{Tr}\hat{g} = +2$) or $\hat{g} = \mathrm{diag}(1,-1,-1,-1)$ (which has $\mathrm{Tr}\hat{g} = -2$). Different choices are encountered throughout the literature.

D. Covariant 3+1 dimensional formulation

Note that "covariant" in this context is not related to our previous discussion of 4-vector components x_μ. Saying that a quantity is Lorentz covariant means that it changes via a Lorentz transformation when going from one inertial frame to another. Scalars and 4-vectors are examples of such quantities. An equation is Lorentz covariant if it may be written with Lorentz covariant quantities.

The second postulate of the special theory of relativity was that the laws of physics should be the same in all inertial frames. Another way to put this is that physical laws have to be Lorentz covariant, i.e. they need to have the same form in all inertial frames. For instance, if a quantity $C_\mu = D_\mu$ in one frame, then $C'_\mu = D'_\mu$ in another frame where the primed quantities are obtained via a Lorentz-transformation.

Let us consider a point in Minkowsi-space with coordinates $\boldsymbol{x} = (x_1, x_2, x_3, x_4)$. A particle moving in this space will be described by a path called a "world line" or *eigenline*. A small change in the coordinates along the eigenline is described by dx_μ. We have seen that $dx_\mu dx_\mu$ is a Lorentz-invariant, in effect it has the same value when measured in any inertial frame. Because of this, we can define the *eigentime* τ as follows:

$$dx_\mu dx_\mu \equiv -c^2 d\tau^2. \tag{7.20}$$

Now, imagine that we attach an inertial system S' to a moving particle. The particle, as seen from S', is then at rest. We obtain

$$dx'_\mu = (0,0,0,\mathrm{i}cdt') \rightarrow dx'_\mu dx'_\mu = -c^2dt^2 \tag{7.21}$$

From the definition of eigentime, we then see that in this case $dt = d\tau$. We can now physically interpret $d\tau$: it is the time measured by a clock moving along with the particle (hence the name eigentime).

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As seen from the stationary inertial frame S, the particle above is moving with velocity u where $u^2 = (dx/dt)^2 + (dy/dt)^2 + (dz/dt)^2$. We obtain

$$dx_\mu = (dx, dy, dz, \mathrm{i}cdt) \tag{7.22}$$
$$\rightarrow dx_\mu dx_\mu = dx^2 + dy^2 + dz^2 - c^2dt^2 \tag{7.23}$$
$$\rightarrow -c^2(d\tau/dt)^2 = u^2 - c^2 \tag{7.24}$$
$$\rightarrow d\tau^2 = (1 - u^2/c^2)dt^2 \tag{7.25}$$
$$\rightarrow dt = \frac{d\tau}{\sqrt{1-\beta^2}} > d\tau. \tag{7.26}$$

This means that the clock in S (where the particle is moving) displays a time dt which is longer than the time $d\tau$ displayed on a watch in S' (where the particle is at rest). This is the relativistic phenomenon of *time dilation*: **moving clocks run slower.**

There exists a similar phenomenon regarding the measurement of lengths in inertial frames that are moving with respect to each other known as *length contraction*: moving objects appear shorter. To see this, consider an object with length L' as measured in a frame S' moving together with the object. In a stationary frame S, we know that the following relation exists between the coordinates z' and z' (assume that the relative motion occurs along the z-axis, without loss of generality): $z' = \gamma(z - vt)$ where v is the relative velocity between S and S'. We know that $L' = z'_2 - z'_1$, which gives the equation

$$L' = \gamma L \tag{7.27}$$

In effect, the object is measured to have a length $L < L'$ and is seen from S as shorter compared its rest-frame length measured in S'.

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81,000 km
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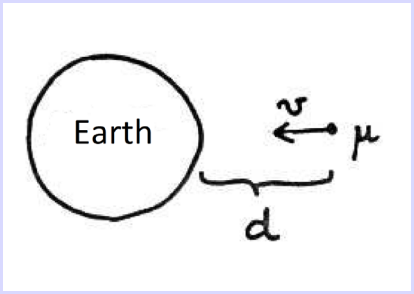
Example 17. Lifetime for muons in the atmosphere. These elementary particles, belonging to the lepton family, are typically created around $d \simeq 6$ km away from Earth via cosmic rays. The lifetime of a muon in its restframe is $\tau = 2 \times 10^{-6}$ s. Its speed relative Earth is $v = 2.994 \times 10^8$ m/s.



Non-relativistically, a muon would thus manage to cover a distance $L_0 = v\tau = 600$ m. This means that no muons should be able to reach the surface of Earth - however, this is in strong disagreement with experimental measurements where many muons are detected. As suspected, we have to treat the problem relativistically due to the high velocities of the muons. We can take two perspectives:

(a) As seen from Earth. The lifetime of the muon is subject to time dilation and its lifetime, as seen from the surface of Earth, becomes $t = \tau/\sqrt{1-(v/c)^2} \simeq 32 \times 10^{-6}$ s. Moving with its speed v it can now cover a distance $L = vt = 9.6$ km $> d$ and thus reach Earth.

(b) As seen from muon. Earth is moving with a relative velocity v toward the muon. But the distance from the muon to Earth, as seen from the muon, is subject to length contraction according to our explanation preceeding this example. Thus, the muon sees a distance $z = z'\sqrt{1-\beta^2} \simeq 375$ m. As a result, Earth reaches the muon after a time $t = z/v \simeq 1.25 \times 10^{-6}$ s $< \tau$, i.e. a shorter time than the muon lifetime. This has been experimentally verified in Bailey et al., Physics Letters **55B**, 420 (1975).

It is important to note that the path element $ds^2 = dx_\mu dx_\mu$ can be both positive, negative, or even zero. We say that a 4-vector x_μ is

- Spacelike if $x_\mu x_\mu > 0$.
- Timelike if $x_\mu x_\mu < 0$.
- Lightlike if $x_\mu x_\mu = 0$.

Note that we are here using x_μ as notation for a 4-vector when it appears isolated, whereas it means the μ-th component when it appears in a summation such as $x_\mu x_\mu$. Now, why these names? To see this, consider two events described by $x_{1\mu} = (\boldsymbol{r}_1, \mathrm{i}ct_1)$ and $x_{2\mu} = (\boldsymbol{r}_2, \mathrm{i}ct_2)$. Consider the difference between these 4-vectors:

$$X_\mu = x_{1\mu} - x_{2\mu} = (\boldsymbol{r}_1 - \boldsymbol{r}_2, \mathrm{i}c(t_1 - t_2)) \tag{7.28}$$

which has the norm

$$X_\mu X_\mu = |\boldsymbol{r}_1 - \boldsymbol{r}_2|^2 - c^2(t_1 - t_2)^2. \tag{7.29}$$

Choose the coordinate systems so that $\boldsymbol{r}_1 - \boldsymbol{r}_2$ is along the z-axis. In a system S' moving with relative velocity v along the z-axis, we have

$$t_1' - t_2' = \gamma[t_1 - t_2 - v(z_1 - z_2)/c^2] = (\gamma/c)[c(t_1 - t_2) - \beta(z_1 - z_2)]. \tag{7.30}$$

If X_μ is space-like, then $X_\mu X_\mu > 0$ which according to the above equation

$$c|t_1 - t_2| < |z_1 - z_2|. \tag{7.31}$$

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In this case, we can always find a velocity $v < c$ in Eq. (7.30) so that $t_1' - t_2' = 0$. In other words, we can always find an inertial frame S' moving with velocity v relative S where the two events are seen as simultaneous. If X_μ is timelike, we have by the same reasoning

$$c|t_1 - t_2| > |z_1 - z_2|. \tag{7.32}$$

meaning that we cannot find an inertial frame S' where the two events occur simultaneously. Events with spacelike separation cannot be connected with a signal moving with the speed of light c, since they can occur simultaneously. Timelike events, on the other hand, can be connected with a signal moving with c so that the two events can influence each other.

Before moving on to discuss relativistic mechanics, we introduce some additional 4-vectors besides the position 4-vector x_μ. The 4-velocity is defined as

$$u_\mu \equiv \frac{dx_\mu}{d\tau}. \tag{7.33}$$

Since x_μ is a 4-vector, u_μ is also a 4-vector since $d\tau$ is a Lorentz-invariant scalar. Since $dx_\mu = (dx_i, \mathrm{i}cdt)$, one obtains

$$u_\mu = \gamma(\boldsymbol{v}, \mathrm{i}c). \tag{7.34}$$

Note that $u_\mu u_\mu = \gamma^2 v^2 - \gamma^2 c^2 = -c^2$.

The 4-current density j_μ is defined as $j_\mu = (\boldsymbol{j}, \mathrm{i}c\rho)$ where $\boldsymbol{j}$ is the current density and ρ is the charge density. The continuity equation, guaranteeing conservation of charge, has the familiar form $\nabla \cdot \boldsymbol{j} = \partial\rho/\partial t = 0$. This can be written compactly with the 4-current density as

$$\frac{\partial}{\partial x_\mu} j_\mu \equiv \partial_\mu j_\mu = 0. \tag{7.35}$$

We note that j_μ is actually the 4-vector $\rho_0 u_\mu$ where ρ_0 is the chage density in the inertial frame where the charges are at rest:

$$j_\mu = \rho_0 u_\mu = (\gamma\rho_0 \boldsymbol{v}, \mathrm{i}c\gamma\rho_0) = (\rho\boldsymbol{v}, \mathrm{i}c\rho) = (\boldsymbol{j}, \mathrm{i}c\rho). \tag{7.36}$$

The charge density ρ for moving charges is larger than ρ_0 due to length contraction: $\rho = \gamma\rho_0 > \rho_0$. The continuity equation is a physical law which should have the same form in all inertial frames, i.e. it should be Lorentz covariant. Let us verify this explicitly. Since $dx_\mu = (\hat{L}^{\mathrm{T}})_{\mu\nu} dx_\nu' = L_{\nu\mu} dx_\nu'$, it follows that

$$\frac{\partial}{\partial x_\nu'} = \frac{\partial x_\mu}{\partial x_\nu'} \frac{\partial}{\partial x_\mu} = L_{\nu\mu} \frac{\partial}{\partial x_\mu}. \tag{7.37}$$

Thus, both $\partial/\partial x_\mu$ and j_μ transform int he same way as dx_μ under a Lorentz-transformation and hence $\partial_\mu j_\mu$ must also be an invariant scalar. The continuity equation is thus Lorentz-covariant.

E. Maxwell's equation, 4-potential, and electromagnetic field tensor

From two of Maxwell's equations, $\nabla \cdot \boldsymbol{B} = 0$ and $\nabla \times \boldsymbol{E} = -\partial\boldsymbol{B}/\partial t$, it follows that we can express the magnetic and electric fields via two potentials $\boldsymbol{A}$ and ϕ as follows:

$$\boldsymbol{B} = \nabla \times \boldsymbol{A},\ \boldsymbol{E} = -\nabla\phi - \partial\boldsymbol{A}/\partial t. \tag{7.38}$$

In vacuum, we have zero electric polarization $\boldsymbol{P}$ and magnetization $\boldsymbol{M}$, which gives $\boldsymbol{D} = \varepsilon_0 \boldsymbol{E}$. From the third of Maxwell's equations, $\nabla \cdot \boldsymbol{D} = \rho$, we get

$$\nabla^2\phi + \frac{\partial}{\partial t}(\nabla \cdot \boldsymbol{A}) = -\rho/\varepsilon_0. \tag{7.39}$$

Moreover, we have that $\boldsymbol{H} = \boldsymbol{B}/\mu_0$, which inserted into Maxwell's fourth and final equation $\nabla \times \boldsymbol{H} = \boldsymbol{j} + \partial\boldsymbol{D}/\partial t$ gives

$$\nabla^2 \boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2 \boldsymbol{A}}{\partial t^2} - \nabla(\nabla \cdot \boldsymbol{A} + \frac{1}{c^2}\frac{\partial\phi}{\partial t}) = -\mu_0 \boldsymbol{j}. \tag{7.40}$$

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Let us take a step back and see what we have accomplished. Maxwell's four equations for $\boldsymbol{E}$ and $\boldsymbol{B}$ in vacuum have now been reduced to two equations for the potentials ϕ and $\boldsymbol{A}$, namely Eqs. (7.39) and (7.40). These equations are coupled, which makes their solution non-trivial. However, it is actually possible to decouple these equations by using the concept of *gauge-invariance*.

To understand gauge-invariance in the context of EM fields, consider that since $\boldsymbol{B} = \nabla \times \boldsymbol{A}$, the physical magnetic field $\boldsymbol{B}$ remains unchanged if we perform the transformation

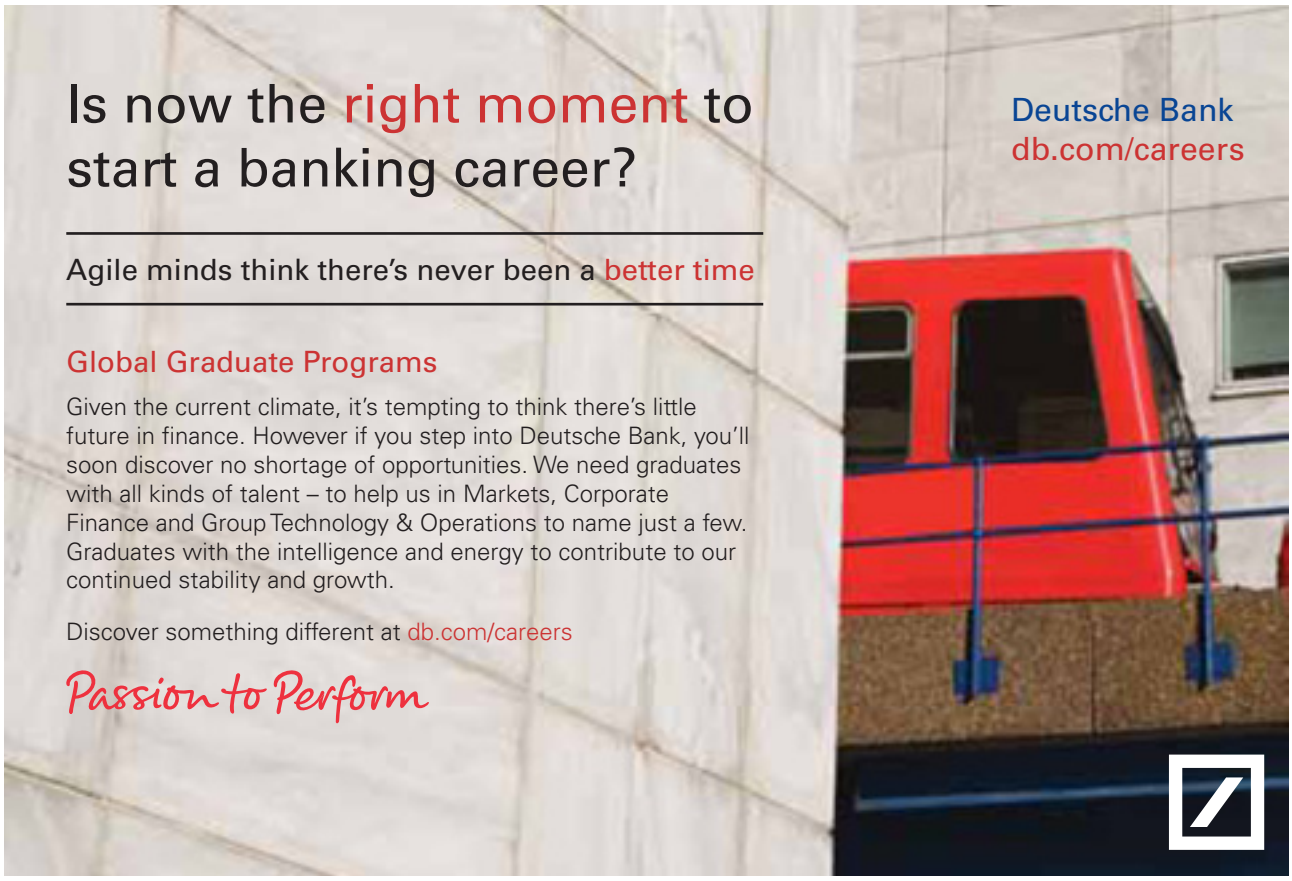
$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \nabla\chi \tag{7.41}$$

where χ is an arbitrary scalar function, since $\nabla \times \nabla\chi = 0$ is an identity. However, in doing this transformation the $\boldsymbol{E}$ field should also be left invariant. Since $\boldsymbol{E} = -\nabla\phi - \partial\boldsymbol{A}/\partial t$, we must therefore simultaneously perform the transformation

$$\phi \to \phi' = \phi - \partial\chi/\partial t. \tag{7.42}$$

This freedom to choose the potentials ϕ and $\boldsymbol{A}$ as we like while keeping the physics intact (invariant fields $\boldsymbol{E}$ and $\boldsymbol{B}$) is known as gauge invariance. We are thus free to choose χ as we like, which can then be utilized to make the equations simpler. For instance, let us choose a χ that satisfies

$$\nabla^2\chi - \frac{1}{c^2}\frac{\partial^2\chi}{\partial t^2} = 0. \tag{7.43}$$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This the so-called Lorenz gauge choice (not *Lorentz*: the gauge choice is due to Ludvig Lorenz, to be distinguished from Hendrik Lorentz). This gauge-choice guarantees us that the so-called Lorenz condition is satisfied:

$$\nabla \cdot \boldsymbol{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0 \tag{7.44}$$

in any inertial frame. You can verify by direct insertion that for this choice of χ, the equation $\nabla \cdot \boldsymbol{A}' + \frac{1}{c^2}\frac{\partial \phi'}{\partial t} = 0$ is also satisfied.

Let us now make use of the Lorenz-condition to decouple the equations for ϕ and $\boldsymbol{A}$ in Eqs. (7.39) and (7.40). We get

$$\begin{aligned} &\nabla^2\phi + \partial(\nabla \cdot \boldsymbol{A})/\partial t = -\rho/\varepsilon_0 \\ \rightarrow &\nabla^2\phi + \frac{\partial}{\partial t}\Big(-\frac{1}{c^2}\frac{\partial \phi}{\partial t}\Big) = -\rho/\varepsilon_0 \\ \rightarrow &(\nabla^2 - \frac{1}{c^2}\partial^2\partial t^2)\phi = -\rho/\varepsilon_0. \end{aligned} \tag{7.45}$$

This is the first equation which now describes ϕ uncoupled from $\boldsymbol{A}$. The second equation is obtain by observing that the second term in Eq. (7.40) is zero due to our Lorenz-gauge choice, so that it becomes

$$(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2})\boldsymbol{A} = -\mu_0 \boldsymbol{j}. \tag{7.46}$$

We now have two decoupled equations for ϕ and $\boldsymbol{A}$. At this point, we introduce the 4-potential

$$A_\mu = (\boldsymbol{A}, \mathrm{i}\phi/c) \tag{7.47}$$

so that the Lorenz-condition reads $\partial_\mu A_\mu = 0$. Now, the two uncoupled wave equations Eqs. (7.45) and (7.46) can be written compactly with 4-vector notation as one single equation

$$\Box^2 A_\mu = -\mu_0 j_\mu. \tag{7.48}$$

Here, we introduced $\Box^2 = \partial_\nu\partial_\nu = \nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$. This is D'Alembert's operator. This is also a Lorentz-covariant equation since A_μ transforms like j_μ while $\Box^2$ is an invariant scalar operator. Hence, Maxwell's electromagnetic theory is covariant.

Let us finally consider how electromagnetic fields transform when changing inertial frame. Consider as before a system S' moving with relative velocity v along the z-axis compared to a stationary system S. We know that the Lorentz-transformation matrix for this scenario reads

$$\hat{L} = L_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \gamma & \mathrm{i}\beta\gamma \\ 0 & 0 & -\mathrm{i}\beta\gamma & \gamma \end{pmatrix}. \tag{7.49}$$

The *electromagnetic field tensor* $F_{\mu\nu}$ is defined as

$$F_{\mu\nu} = \frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu} \equiv A_{\mu,\nu} - A_{\mu,\nu}. \tag{7.50}$$

An important property of this tensor is that it is antisymmetric, meaning $F_{\mu\nu} = -F_{\nu\mu}$. Here, $A_\mu = (\boldsymbol{A}, \mathrm{i}\phi/c)$ is the 4-potential introduced previously. It follows that we can also write

$$F_{\mu\nu} = \begin{pmatrix} 0 & B_3 & -B_2 & -\mathrm{i}E_1/c \\ -B_3 & 0 & B_1 & -\mathrm{i}E_2/c \\ B_2 & -B_1 & 0 & -\mathrm{i}E_3/c \\ \mathrm{i}E_1/c & \mathrm{i}E_2/c & \mathrm{i}E_3/c & 0 \end{pmatrix}. \tag{7.51}$$

The Lorentz-transformation of $F_{\mu\nu}$ reads

$$F'_{\mu\nu} = L_{\mu\alpha}L_{\nu\beta}F_{\alpha\beta}, \tag{7.52}$$

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which is a natural generalization of how the single-indexed 4-vectors transform.

It is particularly instructive to consider the case $v/c \ll 1$, in which case one finds

$$E_1' = E_1 - vB_2,\ E_2' = E_2 + vB_1,\ E_3' = E_3. \tag{7.53}$$

This can be rewritten as

$$\boldsymbol{E}' = \boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}. \tag{7.54}$$

In other words, a particle moving in a constant magnetic field $\boldsymbol{B}$ will experience a net electric field $\boldsymbol{E}'$ even in the absence of any external electric field $\boldsymbol{E}$. A similar transformation equation can be found for the magnetic field

$$\boldsymbol{B}' = \boldsymbol{B} - \frac{1}{c^2}(\boldsymbol{v} \times \boldsymbol{E}). \tag{7.55}$$

We thus see that a particle moving in a constant electric field $\boldsymbol{E}$ will feel a net magnetic field $\boldsymbol{B}'$. As a side-note, this is actually the origin of the spin-orbit interaction in condensed matter physics, which is a relativistic effect. These transformation equations are also used extensively in magnetohydrodynamics.

F. Relativistic mechanics and kinematics

Newton's 2nd law $F = ma$ is invariant under a Galilei-transformation, but not under a Lorentz-transformation. Hence, it is not covariant and cannot be correct in the relativistic case. Thus, we have to find a generalization of this equation which

- Satisfies the criterium of covariance in the special theory of relativity
- Reduces to $\frac{d}{dt}(mv_i) = F_i$ if $v_i \ll c$.

A natural choice is

$$\frac{d}{d\tau}(mu_\mu) = K_\mu \tag{7.56}$$

where m is the invariant mass, τ is the eigentime, u_μ is the 4-velocity, and K_μ is the Minkowski-force. We must demand that K_μ has the property $\lim_{v\to 0} K_i = F_i$ to regain consistency with the non-relativistic limit. Let us use electromagnetic theory as an example since we know that it is Lorentz-covariant and because we know what the force should look like, namely $\boldsymbol{F} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$.

By expressing $\boldsymbol{E}$ and $\boldsymbol{B}$ with their potentials ϕ and $\boldsymbol{A}$, and using that

$$u_\mu A_\mu = \gamma(\boldsymbol{v} \cdot \boldsymbol{A} - \phi), \tag{7.57}$$

one finds that the components of $\boldsymbol{F}$ may be written as:

$$F_i = \frac{q}{\gamma}\Big(\partial_i(u_\mu A_\mu) - \frac{dA_i}{d\tau}\Big). \tag{7.58}$$

Now, both ∂_i and dA_i transform as the space-components of a 4-vector, while $u_\mu A_\mu$ and $d\tau$ are invariant scalars. This allows us to identify $K_i = \gamma F_i$ where:

$$K_i = q\Big(\partial_i(u_\mu A_\mu) - \frac{dA_i}{d\tau}\Big). \tag{7.59}$$

Generalizing this to four dimensions, we then have the Minkowski-force

$$K_\mu = q\Big(\partial_\mu(u_\nu A_\nu) - \frac{dA_\mu}{d\tau}\Big) \tag{7.60}$$

describing the force acting on relativistic, charged particles. The relativistic version of Newton's 2nd law then reads:

$$K_\mu = \frac{dp_\mu}{d\tau} \tag{7.61}$$

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where $p_\mu = mu_\mu$ is the 4-momentum. Thus, $\boldsymbol{F} = d\boldsymbol{p}/dt$ holds also relativistically since $\boldsymbol{K} = d\boldsymbol{p}/d\tau$ and $d\tau = dt/\gamma$. But what does the fourth component of K_μ give us information about? We see that

$$u_\mu K_\mu = u_\mu \frac{d}{d\tau}(mu_\mu) = -\frac{d}{d\tau}(mc^2/2) = 0. \tag{7.62}$$

In effect, $u_i K_i + u_4 K_4 = 0$, providing us with

$$K_4 = \mathrm{i}\gamma \boldsymbol{F} \cdot \boldsymbol{v}/c. \tag{7.63}$$

The components of the Minkowski-force have now all been identified:

$$K_\mu = \gamma(\boldsymbol{F}, \mathrm{i}\boldsymbol{F} \cdot \boldsymbol{v}/c). \tag{7.64}$$

The total relativistic energy is

$$E = \gamma mc^2. \tag{7.65}$$

In the limit $v \ll c$, we may expand $\gamma = 1/\sqrt{1-(v/c)^2}$ in powers of v and one obtains to lowest order:

$$E = mc^2 + \frac{1}{2}mv^2. \tag{7.66}$$

We have regained the familiar kinetic energy, but there is an additional contribution mc^2 that persists even if the particle is at rest ($v = 0$). This is the so-called *rest energy* of a massive particle. If the particle in addition moves in an external potential V, this should be added to E to obtain the total energy.

Let us consider the 4-momentum in some more detail. Just like $x_\mu x_\mu$, $p_\mu p_\mu$ is also an invariant quantity. In general, the so-called contraction of a covariant and contravariant 4-vector $a_\mu b^\mu$ is always a Lorentz-invariant quantity as can be verified by performing the transformation explicitly. For our choice of metric, there is no distinction between covariant and contravariant vectors so that $p_\mu = p^\mu$. Thus, since $p_\mu = (\gamma m\boldsymbol{v}, \mathrm{i}\gamma mc) = (\boldsymbol{p}, \mathrm{i}E/c)$ where $\boldsymbol{p}$ is the relativistic momentum, we get

$$p_\mu p_\mu = p^2 - E^2/c^2 = -(mc^2)^2/c^2 = -m^2c^2. \tag{7.67}$$

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in the rest frame of the particle since then $\boldsymbol{p} = 0$ and $\gamma = 1$. We thus obtain the above expression in the rest frame of the particle, but since it is a Lorentz invariant quantity we know that its value is the same in any inertial frame. Thus, it follows that the following relation holds generally:

$$\boxed{E^2 = p^2c^2 + m^2c^4}.$$

This is the relativistic energy-momentum dispersion relation for a free particle. It has a number of important consequences. For instance, a photon has zero mass $m = 0$ and thus $E = pc$. As a result, it has momentum in spite of being massless. Moreover, since $E = h\nu$ where h is Planck's constant and ν is its frequency, we get $pc = h\nu$ which can be rewritten as

$$p = h/\lambda. \tag{7.68}$$

This is de Broglies formula for the wave-particle dualism.

Example 18. Energy conservation and mass difference. Consider a scenario where two masses m collide and produce a new particle M. In the center of mass frame, the particles must initially move with velocities of equal magnitude but opposite direction, whereas the final particle M must have $v = 0$. Energy and momentum conservation can now be expressed in a single statement: conservation of total 4-momentum p_μ. Now, the total 4-momentum before the collision is

$$P_\mu = p_{1\mu} + p_{2\mu} = (\boldsymbol{p}_1 + \boldsymbol{p}_2, \mathrm{i}E_1/c + \mathrm{i}E_2/c). \tag{7.69}$$

After the collision, we have:

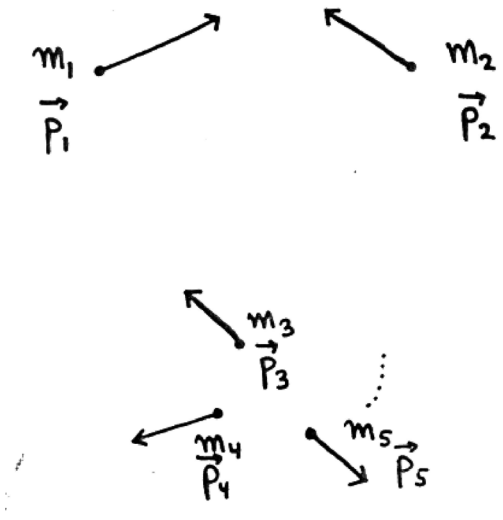
$$P_\mu = (0, \mathrm{i}Mc) \tag{7.70}$$

since M is at rest and thus only has rest energy. It follows that conservation of the fourth component of P_μ (conservation of energy) gives

$$2\gamma mc^2 = Mc^2. \tag{7.71}$$

In effect, $M > 2m$ since $\gamma > 1$. The mass has increased! Relativistically, mass is thus not conserved. The fundamental reason for this is its equivalence to energy via the relation $E = mc^2$ for the rest energy. Kinetic energy before the collision has thus been converted to rest energy, in effect mass.

Another important situation, of particular relevance in high energy physics and particle physics, is where two particles collide/interact and form several new particles (possibly more than 2). We thus have the scenario shown in the figure below.



Without knowing the details of the moment of collision, we can still use classical mechanics on the system a sufficiently long time before and after the collision. It is beneficial to consider this process in the CM frame where the total momentum is $\boldsymbol{P} = 0$ both before and after. Since 4-momentum is conserved (P_μ before, $P'_\mu = P_\mu$ after), we know that

$$P_\mu P_\mu = P'_\mu P'_\mu = (\boldsymbol{P}')^2 + (\mathrm{i}E'/c)^2 = -(E'/c)^2 \equiv -M^2c^2. \tag{7.72}$$

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In the last step, we introduced the so-called *equivalent mass* $M \equiv E'/c$ of the system. It is not equal to the total mass of the particles in general: only in the special case where the momentum of *each of the particles* after the collision is zero (as opposed to the more general statement of their sum being zero) will $M = \sum_r m_r$ where the sum goes over all particles after the collision. This leads us to the important concept of *threshold energy*. The definition of this quantity is that it is the smallest kinetic energy of the initial particles that will enable the reaction to proceed. It corresponds precisely to the case where all masses produced in the collision are at rest afterwards in the center of mass frame: no extra energy has been imparted to give them any kinetic energy.

Let us find an expression for this threshold energy which we denote K_1. We know that

$$P_\mu P_\mu = (p_{1\mu} + p_{2\mu})(p_{1\mu} + p_{2\mu}) = -m_1^2c^2 - m_2^2c^2 + 2(\boldsymbol{p}_1 \cdot \boldsymbol{p}_2 - E_1E_2/c^2) = -M^2c^2. \tag{7.73}$$

But we also know that $P_\mu P_\mu$ is a Lorentz-invariant quantity. Thus, we can compute it in any inertial frame and get the same result. Let us therefore now consider the lab-frame where one particle is at rest to begin with, $\boldsymbol{p}_2 = 0$. This means that $E_2 = m_2c^2$. We obtain

$$M^2c^4 = (m_1^2 + m_2^2)c^4 + 2E_1m_2c^2 = (m_1 + m_2)^2c^4 + 2m_2c(E_1 - m_1c^2). \tag{7.74}$$

Now $E_1 - m_1c^2$ is precisely the kinetic energy of particle 1: its total energy minus its rest mass. It follows that the total kinetic energy before the collision is $K_1 = E_1 - m_1c^2$. From Eq. (7.74), we see that right at the threshold energy (where $M = \sum_r m_r$), we obtain

$$(\sum_r m_r)^2c^4 = (m_1 + m_2)^2c^4 + 2m_2c^2K_1. \tag{7.75}$$

Solving for K_1, we get

$$\frac{K_1}{m_1c^2} = \frac{(\sum_r m_r)^2 - (m_1 + m_2)^2}{2m_1m_2}. \tag{7.76}$$

The Q-value of the reaction is defined as the increase in mass after the collision in the CM-frame:

$$Q = \sum_r m_r - (m_1 + m_2). \tag{7.77}$$

With this definition, we get

$$(\sum_r m_r)^2 - (m_1 + m_2)^2 = Q^2 + 2Q(m_1 + m_2) \tag{7.78}$$

which in terms of the threshold energy then becomes:

$$\frac{K_1}{m_1c^2} = \frac{Q^2 + 2Q(m_1 + m_2)}{2m_1m_2}. \tag{7.79}$$

This equation then expresses the minimum kinetic energy K_1 that must be available initially in order to enable a reaction, as a function of the Q-value (mass increase) of the reaction.

Example 19. Production of antiprotons. Consider the reaction $p + N \to p + N + p + \bar{p}$. Here, N is a nucleon (n or p). The neutron and proton mass are very similar, so that we may set

$$m_p \simeq m_n \simeq m_{\bar{p}} \equiv m = 938 \text{ MeV}/c^2. \tag{7.80}$$

The Q-value is then $4m - 2m = 2m$. The threshold energy then becomes

$$K_1 = 6mc^2, \tag{7.81}$$

which is around 5.57 GeV or $3Qc^2$. In other words, the initial proton must have a kinetic energy of at least $3Q$ in order to enable the reaction when N is at rest.

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However, if we instead consider the CM-frame where $\boldsymbol{p}_1 = -\boldsymbol{p}_2$, one would have found the result $K_1 = K_2 = mc^2 = Qc^2/2$. In other words, the threshold energy for the initial particles is now far less than in the first case. What is the physical reason for this? In the first case where we considered the lab-frame, conservation of momentum dictates that there must be a finite momentum after the reaction. In other words, the initial kinetic energy must be sufficiently high to both produce the rest mass energies of the final particles and to provide them with the required kinetic energy to satisfy momentum conservation. In contrast, if the initial collision takes place in the center of mass frame, there is no requirement that the final particles must have any kinetic energy: they are all allowed to be at rest. In this case, all the initial kinetic energy can be converted to rest mass energy and thus the threshold is lower. This is precisely the reason for why it is beneficial to experimentally accelerate particles in a ring in opposite directions rather than firing particles at a stationary target.

G. The relativity of simultaneity

An important conceptual point regarding relativistic transformations is the *relativity of simultaneity*. In short, this means that two events 1 and 2 that occur simultaneously in one frame ($t_1 = t_2$) do not occur simultaneously in another frame ($t_1' \neq t_2'$) if the two events are separated in space ($\boldsymbol{r}_1 \neq \boldsymbol{r}_2$). This is a key aspect which must be taken into account to avoid inconsistent situations in the special theory of relativity. For instance, we have stated that moving clocks run slower. But that would mean that two persons moving relative each other would both conclude that the other person's clock runs slower, which seems strange. How does one resolve such an apparent paradox? The answer is that one must take into account the relativity of simultaneity.

Let us try to illustrate this with a simple example. Imagine that you have two clocks that are separated by a distance L. We now want to synchronize the clocks, i.e. making sure they start at the same time, by emitting a flash of light from a bulb positioned at the midpoint of the two clocks. This is fine if the system is stationary, but imagine now that the entire arrangement (both clocks and the bulb at the midpoint) is on a bus and thus moving with a velocity v. For a stationary observer, it is clear that the flash of light will take longer to reach the clock to the right since it is moving away from the bulb, whereas the flash of light will take a shorter amount of time to reach the clock to the left since it is moving toward the bulb. A stationary observer is thus exposed to two relativistic effects due to the moving clocks:

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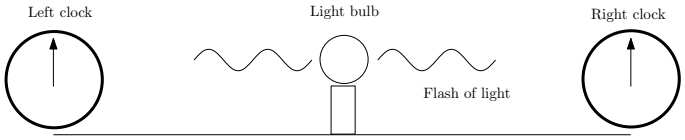
- Both clocks will run slower than his clock by a factor $\sqrt{1-(v/c)^2}$ since they are moving: this is the phenomenon of time-dilation.
- But there is an additional effect: the two clocks are not synchronized as seen from the stationary frame (even if they started at the same time as seen from the bus). In fact, one can show that he will see the left clock reading vL/c^2 seconds at the moment the flash of light reaches the right clock, causing it to start running.

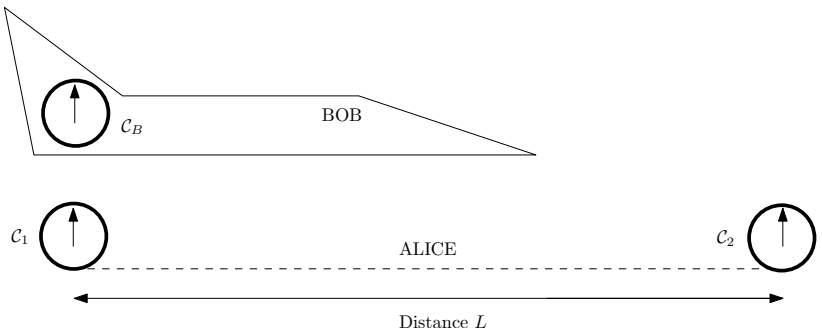
So the clocks on the bus, as seen from the stationary observer, run slower but are also not synchronized.



Taking this into account, we can now show why two observers moving relative each other can both conclude that the other person's clock is running slower - and both be right! The following example is a rewritten version of "Time Dilation: A Worked Example" given by M. Fowler, UVa Physics. Consider the frame of Alice where there are two synchronized clocks $\mathcal{C}_1$ and $\mathcal{C}_2$ that are separated by a distance L. Now, Bob has a very fast airplane and flies by at a speed of $0.8c$ (see figure below). Bob has a clock $\mathcal{C}_B$ on his airplane which starts at the same time as $\mathcal{C}_1$, i..e. $\mathcal{C}_1$ and $\mathcal{C}_B$ are synchronized. Alice would measure that the airplane requires a time of $t = L/0.8c$ to travel from $\mathcal{C}_1$ to $\mathcal{C}_2$. Bob's clock, which is moving relative Alice, would be subject to time dilation and should thus show a time $t_B = t\sqrt{1-(v/c)^2} = 0.6t$.

So, at the moment when Bob passes by the clock $\mathcal{C}_2$ both Alice and Bob will agree that $\mathcal{C}_2$ shows a time t whereas $\mathcal{C}_B$ shows a time $0.6t$. In effect, Bob's clock is running slower, which Alice is perfectly happy with since she knows that moving clocks run slower. But what about Bob? How is this consistent with the fact that according to Bob, it is Alice's clock that should be running slower since she is moving relative him?

This is exactly where the relativity of simultaneity comes into play. The clock $\mathcal{C}_1$, which is synchronized with $\mathcal{C}_B$, is indeed running slower than $\mathcal{C}_B$. In fact, since $\mathcal{C}_B$ is showing the time $0.6t$, $\mathcal{C}_1$ should be showing the time $0.6^2t = 0.36t$. But $\mathcal{C}_2$ should not display this time, because as seen from Bob, $\mathcal{C}_2$ *is not synchronized with* $\mathcal{C}_1$. Due to the reasoning presented in the initial example with the lightbulb on the bus, $\mathcal{C}_1$ is behind $\mathcal{C}_2$ by $Lv/c^2 = 0.8L/c$ seconds. Bob can thus safely state that $\mathcal{C}_1$ is indeed running slow compared to $\mathcal{C}_B$ as he passes the clock $\mathcal{C}_2$, whereas Alice can safely state that $\mathcal{C}_B$ is running slow compared to her clock $\mathcal{C}_2$ as Bob flies by.



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VIII. CANONICAL TRANSFORMATIONS

Youtube-videos. 44-51 in this playlist.

Learning goals. After reading this chapter, the student should:

- Be familiar with phase space and the equivalence between Lagrange's and Hamiltons's formulations
- Understand how Hamilton's equations can be derived from a modified Hamilton's principle
- Understand how canonical transformations are derived from a generating function
- Know Poisson brackets, and the related Jacobi's identity and Poisson's theorem
- Know Liouville's theorem
- Know the essentials of the Hamilton-Jacobi theory

Canonical transformations are related the Hamiltonian formulation of mechanics. We saw in Chapter III that it is usually *not* an advantage to use the Hamiltonian formalism instead of the Lagrangian formalism when solving specific problems in mechanics. The advantages with the Hamiltonian formalism are of a more fundamental kind, namely that the coordinates q and the momenta p are considered to be independent variables *on the same level*. This is quite an important point, especially in statistical mechanics and in quantum mechanics.

A. Transformation of phase space

The **phase space** is spanned by $2n$ axes; n axes for q_i and n axes for p_i. We remember that canonical momentum was given by

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = p(q, \dot{q}, t), \qquad i \in \{1, 2, ..., n\},$$

and Hamilton's equations were

$$\left.\begin{aligned} \dot{q}_i &= \tfrac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\tfrac{\partial H}{\partial q_i} \end{aligned}\right\}; \qquad i = 1, 2, ..., n.$$

We have already seen that we can perform "usual" coordinate transformations,

$$Q_i = Q_i(q, t)$$

for example from Cartesian coordinates $q = \{x, y\}$ to plane polar coordinates, $q = \{r, \vartheta\}$. A transformation of this kind is called a **point transformation**. More generally, and still in accordance with the Hamiltonian formulation, we can transform both q_i and p_i, implying a transformation of the phase space:

$$\begin{aligned} Q_i &= Q_i(q, p, t) \\ P_i &= P_i(q, p, t). \end{aligned}$$

Here Q_i and P_i are canonical coordinates which satisfy the "Hamiltonian equations":

$$\boxed{\begin{aligned} \dot{Q}_i &= \tfrac{\partial K}{\partial P_i} \\ \dot{P}_i &= -\tfrac{\partial K}{\partial Q_i}. \end{aligned}} \tag{8.1}$$

The function $K(Q, P, t)$ is the Hamiltonian in the new coordinates, and (8.1) is a **canonical transformation**.

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We remember from Chapter II that Lagrange's equations can be derived from Hamilton's principle:

$$\delta\int_{t_1}^{t_2} L(q,\dot{q},t)dt = 0.$$

Correspondingly, Hamilton's equations be derived from a **modified Hamilton's principle**:

$$\delta\int_{t_1}^{t_2} [p_i\dot{q}_i - H(p,q,t)]dt = 0. \tag{8.2}$$

This can be seen by starting from the variational principle

$$\delta I = \delta\int_{t_1}^{t_2} f(q,\dot{q},p,t)dt \equiv \delta\int_{t_1}^{t_2} [p_i\dot{q}_i - H(p,q,t)]dt = 0,$$

in which p_i and q_i are looked upon as independent coordinates. Note that $f(q,\dot{q},p,t) = p_iq_i - H(p,q,t)$ does not contain $\dot{p}_i$. The variational principle $\delta I = 0$ thus leads, as we have seen, to the Euler equations for f, under the condition that we can set the boundary terms at $t = t_1, t_2$ equal to 0. This is straightforward for the coordinates q_i:

$$\left[\frac{\partial f}{\partial \dot{q}_i}\delta q_i\right]_{t_1}^{t_2} = 0,$$

because $\delta q_i(t_1) = \delta q_i(t_2) = 0$. We need however also the property

$$\left[\frac{\partial f}{\partial \dot{p}_i}\delta p_i\right]_{t_1}^{t_2} = 0.$$

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Why is this true, since there is no condition on δp_i at the end points? The explanation is that the function f does not contain $\dot{p}$, what implies $\frac{\partial f}{\partial \dot{p}} = 0$; cf. the expression for f above. The last equation is thus satisfied after all. We then obtain the Euler equations for f, which are the same as the usual Hamilton equations:

$$\frac{d}{dt}\frac{\partial f}{\partial \dot{q}_i} - \frac{\partial f}{\partial q_i} = 0 \;\Rightarrow\; \dot{p}_i + \frac{\partial H}{\partial q_i} = 0$$

$$\frac{d}{dt}\underbrace{\frac{\partial f}{\partial \dot{p}_i}}_{=0} - \frac{\partial f}{\partial p_i} = 0 \;\Rightarrow\; \dot{q}_i - \frac{\partial H}{\partial p_i} = 0.$$

Since Hamilton's equations are satisfied also for P and Q, the modified Hamilton's principle has to hold also in this case:

$$\delta\int_{t_1}^{t_2} [P_i\dot{Q}_i - K(P,Q,t)]dt = 0.$$

We compare with (8.2), and see that

$$\boxed{p_i\dot{q}_i - H = P_iQ_i - K + \tfrac{dF}{dt}, \text{ where } \delta F(t_1) = \delta F(t_2) = 0.} \tag{8.3}$$

Here the new function F is *arbitrary* function, except that it has zero variation in the end points. Therefore dF/dt does not contribute to the integral.

Canonical transformations are useful in practice if F contains half of the variables from the old set and half from the new. One then calls F a **generating function**; it acts as a "bridge" between the sets (q,p) and (Q,P). When choosing the function F there are four possible alternatives which we will consider successively.

1. Alternative 1: $F = F_1(q,Q,t)$

This choice leads to

$$\begin{aligned} p_i\dot{q}_i - H &= P_iQ_i - K + \frac{dF_1}{dt} \\ &= P_iQ_i - K + \frac{\partial F_1}{\partial t} + \frac{\partial F_1}{\partial q_i}\dot{q}_i + \frac{\partial F_1}{\partial Q_i}\dot{Q}_i \end{aligned}$$

Since q_i and Q_i are considered independent, this equation is satisfied identically only if

$$\begin{aligned} p_i &= \tfrac{\partial F_1}{\partial q_i} \\ P_i &= -\tfrac{\partial F_1}{\partial Q_i} \\ \underline{K} &\underline{= H + \tfrac{\partial F_1}{\partial t}.} \end{aligned} \tag{8.4}$$

2. Alternative 2: $F = F_2(q,P,t) - Q_iP_i$

We now get

$$\begin{aligned} p_i\dot{q}_i - H &= P_i\dot{Q}_i - K + \frac{dF_2}{dt} - \dot{Q}_iP_i - Q_i\dot{P}_i \\ &= -K + \frac{\partial F_2}{\partial t} + \frac{\partial F_2}{\partial q_i}\dot{q}_i + \frac{\partial F_2}{\partial P_1}\dot{P}_i - Q_i\dot{P}_i. \end{aligned}$$

In this case q_i and P_i are considered as independent coordinates, so that we obtain

$$\begin{aligned} p_i &= \tfrac{\partial F_2}{\partial q_i} \\ Q_i &= \tfrac{\partial F_2}{\partial P_i} \\ \underline{K} &\underline{= H + \tfrac{\partial F_2}{\partial t}.} \end{aligned} \tag{8.5}$$

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Note that $F_1(q, Q, t)$ and $F_2(q, P, t)$ are related via the Legendre transformation (with $P_i = -\frac{\partial F_1}{\partial Q_i}$):

$$F_1 = -P_i Q_i + \underbrace{F_2(q, P, t)}_{\text{“Integration constant.”}}$$

This means that the coordinate P is left out and Q comes in (or vice versa).

3. Alternative 3: $F = q_i p_1 + F_3(p, Q, t)$

The third possible choice is $F = q_i p_1 + F_3(p, Q, t)$. From

$$p_1 \dot{q}_i - H = P_i \dot{Q}_i - K + \frac{dF_3}{dt},$$

we get

$$p_i \dot{q}_i - H = P_i \dot{Q}_i - K + p_i \dot{q}_i + \dot{p}_i q_i + \frac{d}{dt} F_3(p, Q, t)$$
$$-\dot{p}_i q_i - H = P_i \dot{Q}_i - K + \frac{\partial F_3}{\partial t} + \frac{\partial F_3}{\partial p_i} \dot{p}_i + \frac{\partial F_3}{\partial Q_i} \dot{Q}_i.$$

As in this case p_i are Q_i independent, we get in the same way as above:

$$\begin{aligned} q_i &= -\tfrac{\partial F_3}{\partial p_i} \\ P_i &= -\tfrac{\partial F_3}{\partial Q_i} \\ K &= H + \tfrac{\partial F_3}{\partial t}. \end{aligned} \tag{8.6}$$

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4. Alternative 4: $F = q_i p_1 - Q_i P_i + F_4(p, P, t)$

The same procedure as above gives now

$$p_i\dot{q}_i - H = P_i\dot{Q}_i - K + p_i\dot{q}_i + \dot{p}_i q_i - P_i\dot{Q}_i - \dot{P}_i Q_i + \frac{d}{dt}F_4(p, P, t)$$
$$-\dot{p}_i q_i - H = -Q_i\dot{P}_i - K + \frac{\partial F_4}{\partial t} + \frac{\partial F_4}{\partial p_i}\dot{p}_i + \frac{\partial F_4}{\partial P_i}\dot{P}_i,$$

and as above, since p_i and P_i are independent we get

$$\begin{aligned} q_i &= -\tfrac{\partial F_4}{\partial p_i} \\ Q_i &= \tfrac{\partial F_4}{\partial P_i} \\ K &= H + \tfrac{\partial F_4}{\partial t}. \end{aligned} \tag{8.7}$$

Example 20. General transformation. Consider a transformation of type 2 above, given by $F_2 = q_i P_i$. It gives us

$$p_i = \frac{\partial F_2}{\partial q_i} = P_i; \qquad Q_i = \frac{\partial F_i}{\partial P_i} = q_i; \qquad K = H.$$

The function F_2 thus generates the identity transformation!
To make it a little more general, let $F_2 = f_i(q_1, q_2, ..., q_n, t) \cdot P_i$, whereby we get

$$Q_i = \frac{\partial F_2}{\partial P_i} = f_i(q, t).$$

The new coordinates depend only on the old coordinates and the time, not on the momenta. The transformation is of the type $Q_i = Q_i(q, t)$, i.e. a point transformation. Thus, a point transformation is a special case of a canonical transformation.

Example 21. Harmonic oscillator. We start with $H = p^2/2m + kq^2/2$ in "usual" coordinates (one dimension). With $\omega^2 = k/m$ we can write

$$H = \frac{1}{2m}(p^2 + m^2\omega^2 q^2).$$

If we can find a transformation

$$p = f(P)\cos Q; \qquad q = \frac{f(P)}{m\omega}\sin Q,$$

the $K = H$ becomes cyclic in the new coordinate Q:

$$K = H = \frac{f^2(P)}{2m}(\cos^2 Q + \sin^2 Q) = \frac{f^2(P)}{2m}.$$

We must determine $f(P)$ such that the transformation becomes canonical. With the transformation above:

$$p = m\omega p \cdot \cot Q, \qquad \text{[independent of} f(P).]$$

This corresponds to F of the type $F_1(q, Q)$:

$$p = -\frac{\partial}{\partial q}F_1(q, Q) \Longrightarrow F_1 = \frac{1}{2}m\omega q^2 \cot Q \qquad \text{(simplest solution).}$$

The other half of the transformation is

$$P = -\frac{\partial F_1}{\partial Q} = \frac{m\omega q^2}{2\sin^2 Q} \Longrightarrow q = \sqrt{\frac{2P}{m\omega}}\sin Q.$$

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A comparison with the original transformation equations gives:

$$f(P) = \sqrt{2m\omega P}, \Longrightarrow H = \frac{f^2(P)}{2m} = \omega P$$

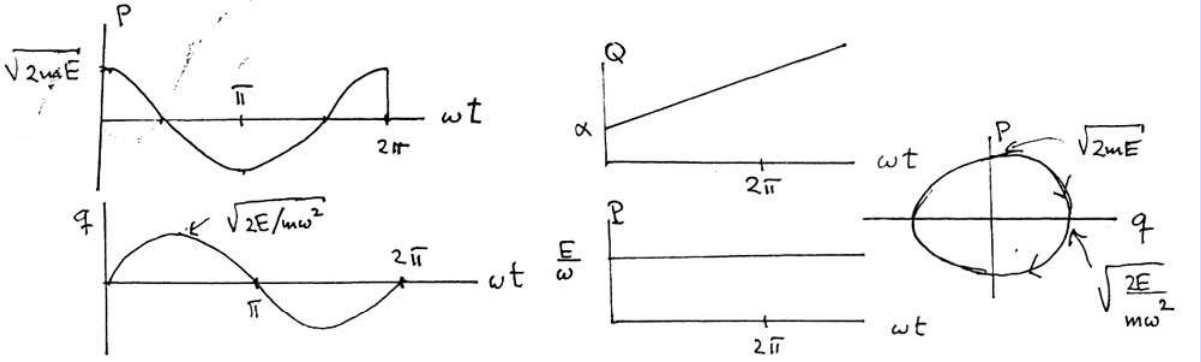
expressed in terms of the transformed variables. Since Q is a cyclic coordinate, the conjugate momentum P has to be a constant. Thus we have learned that $H = E =$ total energy $=$ constant, and we get $P = E/\omega$.
The equation of motion for Q becomes

$$\dot{Q} = \frac{\partial H}{\partial P} = \omega \Longrightarrow Q(t) = \omega t + \alpha \qquad (\alpha \text{ to be determined by the initial conditions}).$$

The solution for q becomes

$$q = \sqrt{\frac{2P}{m\omega}} \sin Q = \sqrt{\frac{2E}{m\omega^2}} \sin(\omega t + \alpha),$$

which we recognize as the usual solution for a harmonic oscillator.



B. Poisson brackets

The Poisson bracket of two functions u and v with respect to canonical variables q and p is defined as

$$[u, v]_{q,p} = \sum_{i=1}^{n} \left(\frac{\partial u}{\partial q_i} \frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i} \frac{\partial v}{\partial q_i} \right). \tag{8.8}$$

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One sees that

$$[u, v]_{q,p} = -[v, u]_{q,p} . \tag{8.9}$$

Moreover it is evident that the following relations hold:

$$[u, C]_{q,p} = 0 \qquad \text{when } C \text{ is const.} \tag{8.10}$$
$$[q_i, q_j]_{q,p} = [p_i, p_j]_{q,p} = 0 \tag{8.11}$$
$$[q_i, p_j]_{q,p} = \delta_{ij}. \tag{8.12}$$

Let $F = F(q_i, p_i, t)$ be an arbitrary function expressed in terms of canonical variables q_i, p_i. Then

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial F}{\partial q_i}\dot{q}_i + \frac{\partial F}{\partial p_i}\dot{p}_i \right) = \frac{\partial F}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial F}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial q_i} \right),$$

where we have made use of Hamilton's equations. Thus

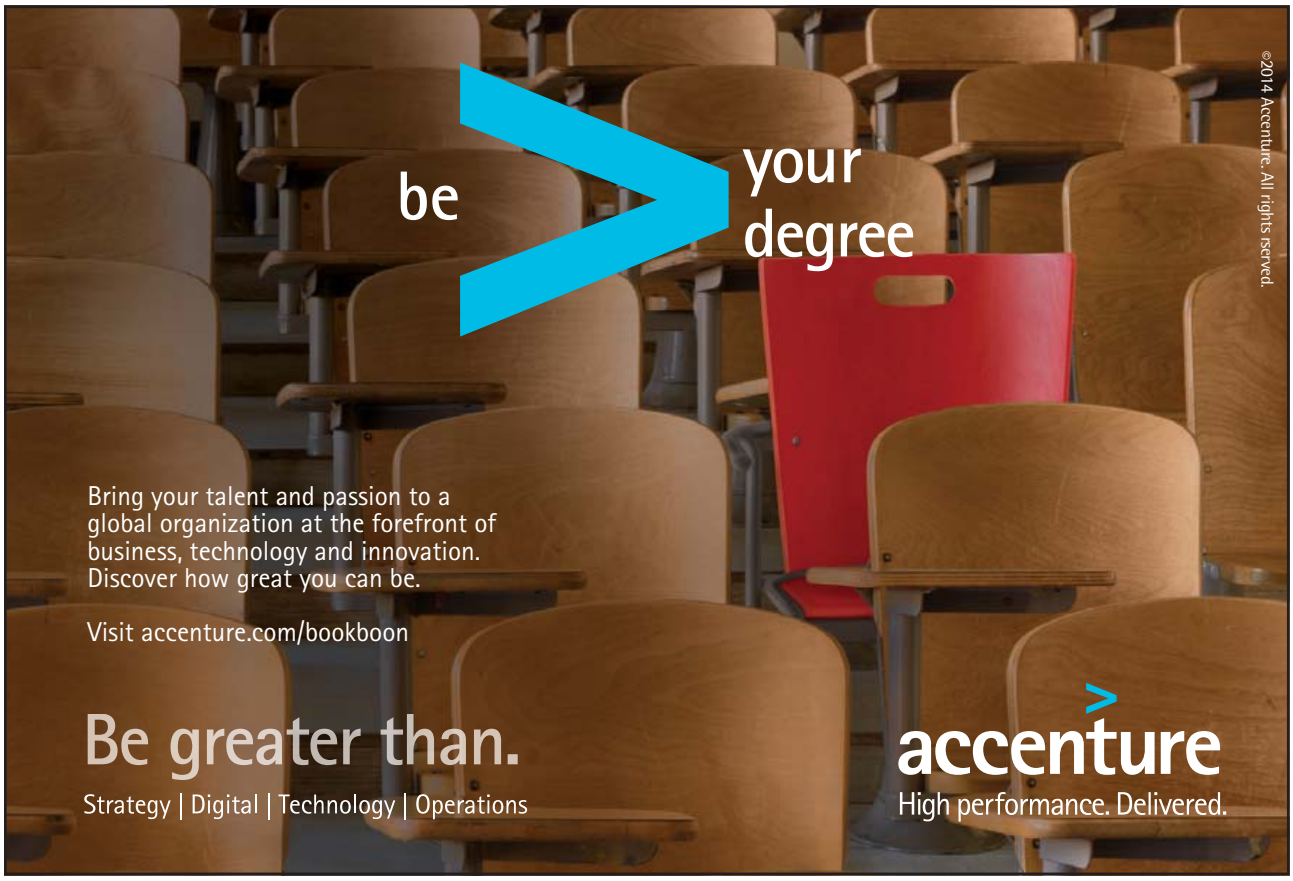
$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + [F, H]_{q,p} . \tag{8.13}$$

If F is a constant of motion, $dF/dt = 0$, one thus has

$$\frac{\partial F}{\partial t} + [F, H]_{q,p} .$$

In other words, if F does not depend explicitly on t, the condition that F is a constant of motion is that

$$[F, H]_{q,p} = 0.$$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Other formal properties of the Poisson brackets are the following:

$$[u_1 + u_2, v]_{q,p} = [u_1, v]_{q,p} + [u_2, v]_{q,p} \tag{8.14}$$

$$[u_1 u_2, v]_{q,p} = u_1 [u_2, v]_{q,p} + u_2 [u_1, v]_{p,q} \tag{8.15}$$

$$\frac{\partial}{\partial t}[u, v]_{p,q} = \left[\frac{\partial u}{\partial t}, v\right]_{p,q} + \left[u, \frac{\partial v}{\partial t}\right]_{p,q} \tag{8.16}$$

1. Connection with quantum mechanics

In quantum mechanics a commutator between two operators u and v (remember that a function can also be regarded as an operator) is defined as

$$[u, v] = uv - vu.$$

The quantum mechanical property

$$[q_i, p_j] = i\hbar\delta_{ij}$$

should be well known. Together with the relation we found, $[q_i, p_j]_{q,p} = \delta_{ij}$, it seems natural to assume that the connection between quantum mechanical commutators and Poisson brackets is

$$[u, v] = i\hbar [u, v]_{q,p}\,. \tag{8.17}$$

A somewhat closer justification can be given by comparing Heisenberg's operator equation in quantum mechanics

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{1}{i\hbar}[A, H]\,,$$

with equation 8.13. The equations take the same form if

$$\frac{1}{i\hbar}[A, H] \leftrightarrow [F, H]_{q,p}\,.$$

2. Jacobi's identity and Poisson's theorem

We will only mention (not derive in detail) these results. From now on we drop the subscript $_{q,p}$. **Jacobi's identity** reads

$$[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0. \tag{8.18}$$

This identity is actually made use of quite often in quantum mechanics (whoever has time and interest, can himself insert the definition of Poisson brackets in the expression on the left hand side and verify that the identity is right).

Moreover, **Poisson's theorem** reads:

If F and G are two constants of motion that do not depend on time explicitly, then the Poisson bracket $[F, G]$ will also be a constant of motion.

Proof. Insert $w = H$ in Jacobi's identity:

$$[H, [F, G]] + [G, [H, F]] + [F, [G, H]] = 0.$$

Since F and G are constants of motion and not explicitly time dependent, one has $[H, G] = 0$ and $[H, F] = 0$ from equation 8.13. Accordingly

$$[H, [F, G]] = 0,$$

which (again from equation (8.13) implies that $[F, G]$ has to be a constant of motion. This completes the proof. □

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Example 22. Poisson's bracket between momentum and angular momentum. We want to find Poisson brackets made from the Cartesian components of the momentum vector $\vec{p}$ and the angular momentum vector $\vec{L} = \vec{r} \times \vec{p}$ for a particle. Consider

$$[p_x, L_x] = [p_x, yp_z - zp_y] = [p_x, y]\, p_z - [p_x, z]\, p_y,$$

because $[p_i, p_k] = 0$. As $[p_i, x_k] = \delta_{ik}$, one has $[p_x, y] = 0$, $[p_x, z] = 0$ and thus $[p_x, L_x] = 0$. Just the same would of course hold if we had replaced x with y or z. We consider further two different components, for instance

$$[p_x, L_y] = [p_x, zp_x - xp_z] = \underbrace{[p_x, z]}_{=0} p_x - [p_x, x]\, p_z = + \underbrace{[x, p_x]}_{=1} p_z = p_z.$$

A cyclic interchange of the coordinates x, y, z above gives us

$$[p_y, L_z] = p_x, \qquad [p_z, L_x] = p_y.$$

Altogether:

$$[p_i, L_j] = \epsilon_{ijk} p_k.$$

Alternatively, we can express the above results in a more compact form:

$$[p_i, L_j] = [p_i, \epsilon_{jlm} x_l p_m] = \underbrace{[p_i, x_l]}_{=-\delta_{il}} \epsilon_{jlm} p_m = -\epsilon_{jim} p_m = \epsilon_{ijk} p_k.$$

Correspondingly, we find

$$[x_i, L_j] = [x_i, \epsilon_{jlm} x_l p_m] = \underbrace{[x_i, p_m]}_{=-\delta_{im}} \epsilon_{jlm} x_l = \epsilon_{jli} x_l = \epsilon_{ijk} x_k.$$

Example 23. Poisson brackets between angular momentum components. We intend to find the Poisson brackets between angular momentum components. With use of the summation convention we can calculate directly

$$[L_x, L_y] = \frac{\partial L_x}{\partial x_i} \frac{\partial L_y}{\partial p_i} - \frac{\partial L_x}{\partial p_i} \frac{\partial L_y}{\partial x_i}, \qquad i \in \{1, 2, 3\}.$$

Here

$$\begin{aligned}
\frac{\partial L_x}{\partial x_i} &= \frac{\partial}{\partial x_i} (yp_z - zp_y) = \delta_{yi} p_z - \delta_{zi} p_y \\
\frac{\partial L_y}{\partial p_i} &= \frac{\partial}{\partial p_i} (zp_x - xp_z) = z\delta_{xi} - x\delta_{zi} \\
\frac{\partial L_x}{\partial p_i} &= \frac{\partial}{\partial p_i} (yp_z - zp_y) = y\delta_{zi} - z\delta_{yi} \\
\frac{\partial L_y}{\partial x_i} &= \frac{\partial}{\partial x_i} (zp_x - xp_z) = \delta_{zi} p_x - \delta_{xi} p_z,
\end{aligned}$$

which gives

$$[L_x, L_y] = (\delta_{yi} p_z - \delta_{zi} p_y)(z\delta_{xi} - x\delta_{zi}) - (y\delta_{zi} - z\delta_{yi})(\delta_{zi} p_x - \delta_{xi} p_z) = xp_y - yp_x = L_z.$$

The generalized version of this is (we do not give all details here):

$$[L_i, L_j] = \epsilon_{ijk} L_k.$$

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The equation

$$[L_i, L_j] = \epsilon_{ijk} L_k \tag{8.19}$$

is another example of the relation to quantum mechanics, since a closely similar relation (except from a factor $i\hbar$) defines the algebra for angular momentum operators. One says that generators G_i for a Lie-group generally satisfy the relation

$$[G_i, G_j] = C_{ijk} G_k, \tag{8.20}$$

where C_{ijk} are called the structure coefficients. In our case the rotation group in three dimensions is called SO(3), and $C_{ijk} = \epsilon_{ijk}$.

3. Canonical transformation of Poisson brackets

Poisson brackets are invariant under a canonical transformation:

$$[u, v]_{q,p} = [u, v]_{Q,P}\,. \tag{8.21}$$

This can be easily seen for the harmonic oscillator, where

$$q = \sqrt{\frac{2P}{m\omega}} \sin Q, \qquad p = m\omega q \cot Q, \qquad P = E/\omega.$$

4. Liouville's theorem

The phase space is spanned by the p_i and q_i axes. A point in the phase space corresponds to a definite state of the physical system. When the system develops in time, this point describes a so-called phase path.

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Liouville's theorem reads:

Let $d\Gamma = dq_1 \cdots dq_n \cdot dp_1 \cdots dp_n$ be a volume element in the phase space. Under a canonical transformation an arbitrary volume of the phase space will be invariant:

$$\int dq_1 \cdots dq_n \cdot dp_1 \cdots dp_n = \int dQ_1 \cdots dQ_n \cdot dP_1 \cdots dP_n. \tag{8.22}$$

Proof. Under a transformation of variables in a multiple integral will generally

$$\int dQ_1 \cdots dQ_n \cdot dP_1 \cdots dP_n = \int D \cdot dq_1 \cdots dq_n \cdot dp_1 \cdots dp_n,$$

where

$$D \equiv \frac{\partial(Q_1 ... Q_n, P_1 ... P_n)}{\partial(q_1 ... q_n, p_1 ... p_n)}$$

is the **Jacobi determinant**. We have to show that for any canonical transformation one has $D = 1$. Mathematically, we can handle the Jacobi determinant as a fraction:

$$D = \frac{\frac{\partial(Q_1 ... Q_n, P_1 ... P_n)}{\partial(q_1 ... q_n, P_1 ... P_n)}}{\frac{\partial(q_1 ... q_n, p_1 ... p_n)}{\partial(q_1 ... q_n, P_1 ... P_n)}} = \frac{\left.\frac{\partial(Q_1 ... Q_n)}{\partial(q_1 ... q_n)}\right|_{P=\text{const.}}}{\left.\frac{\partial(p_1 ... p_n)}{\partial(P_1 ... P_n)}\right|_{q=\text{const.}}}.$$

We assume now the alternative 2 listed under canonical transformations, i.e. $F_2 = F_2(q_i, P_i)$. We then have $p_i = \frac{\partial F_2}{\partial q_i}$, $Q_i = \frac{\partial F_2}{\partial P_i}$. Consider the ik-element in the numerator:

$$\left(\frac{\partial Q_i}{\partial q_k}\right)_P = \frac{\partial}{\partial q_k}\frac{\partial F_2}{\partial P_i},$$

and likewise the ik-element in the denominator:

$$\left(\frac{\partial p_i}{\partial P_k}\right)_q = \frac{\partial}{\partial P_k}\frac{\partial F_2}{\partial q_i}.$$

Since a determinant is independent under an interchange of rows and columns, $(i \leftrightarrow k)$, one gets $D = 1$ under a canonical transformation, as advertised. □

We have seen that the time development of the system can be described as a canonical transformation. Since the phase space is conserved under a canonical transformation, it follows that the phase volume is a constant.

C. Hamilton-Jacobi theory

Canonical transformations can be used to solve mechanical problems. What one wishes to find, by using canonical transformations as a tool, are new coordinates that are cyclic. With cyclic coordinates the integration of the equations of motion (as we have seen several times already) can often be trivial.

One obtains automatically new variables that are constants by requiring that that the transformed Hamilton function K should be equal to zero. The canonical equations then become

$$\dot{Q}_i = \frac{\partial K}{\partial P_i} = 0$$
$$\dot{P}_i = -\frac{\partial K}{\partial Q_i} = 0.$$

Here K is related to the generating function F via

$$K = H + \frac{\partial F}{\partial t},$$

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which with $K = 0$ gives us

$$H(p, q, t) + \frac{\partial F}{\partial t} = 0.$$

It turns out to be convenient to choose the solution $F = F_2 = F_2(q, P, t)$. We make use of the equation (8.5), $p_i = \partial F_2/\partial q_i$, and change the notation by redubbing $F_2 \to S$. The result becomes

$$H(q_1, ..., q_n, \frac{\partial S}{\partial q_1}, ..., \frac{\partial S}{\partial q_n}, t) + \frac{\partial S}{\partial t} = 0, \tag{8.23}$$

which is called the **Hamilton-Jacobi equation**.

The Hamilton-Jacobi equation is a first order partial differential equation with $n + 1$ variables, namely $q_1, ..., q_n$ and t, for the generating function S. The S is called **Hamilton's principal function**.
We know that the new momenta are constants (we have transformed the problem to a phase space, i.e. a canonical set of coordinates):

$$P_i \equiv \alpha_i = \text{const.}.$$

We assume a solution of the form

$$S = S(q_1, ..., q_n, \alpha_1, ..., \alpha_{n+1}, t),$$

where $\alpha_1, ..., \alpha_{n+1}$ are mathematically speaking $n + 1$ independent constants of integration. Since S itself does not occur in (8.23), will $S + \alpha$, with α an arbitrary constant, also be a solution. This has to correspond to one of the $n + 1$ solutions, and is of no physical significance since S only occurs in (8.23) in the form of derivatives. For our purpose it is sufficient to write the solution in the form

$$S = S(q_1, ..., q_n, \alpha_1, ..., \alpha_n, t).$$

We can now *choose* the n integration constants equal to the new constant momenta $P_i \equiv \alpha_i$. We thus have

$$p_i = \frac{\partial}{\partial q_i} S(q, \alpha, t), \tag{8.24}$$

as the first part of the transformation equations. The second half of the transformation equations between old and new coordinates, (8.5), is

$$Q_i = \frac{\partial}{\partial \alpha_i} S(q, \alpha, t) \equiv \beta_i. \tag{8.25}$$

We assume finally that this equation is solved with respect to the original coordinates, so that

$$q_i = q_i(\alpha, \beta, t). \tag{8.26}$$

When viewed mathematically, these equations demonstrate the equivalence between

- the equations with which we started, namely $2n$ canonical equations of motion (first order differential equations), and
- the first order partial Hamilton-Jacobi differential equation.

General procedure of solution

Let us summarize the general procedure of solution given above:

1. From a known Hamilton function H, we construct the Hamilton-Jacobi equation,

$$H + \frac{\partial S}{\partial t} = 0,$$

and find the solution $S = S(q, \alpha, t)$ for Hamilton's principal function S.

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2. Thereafter we find

$$Q_i = \frac{\partial}{\partial \alpha_i} S(q, \alpha, t) \equiv \beta_i,$$

and from that again

$$q_i = q_i(\alpha, \beta, t).$$

3. Finally we find the original momenta,

$$p_i = \frac{\partial}{\partial q_i} S(q, \alpha, t).$$

A simplification can here be done if H does not contain t explicitly (conservative system). Then we can write

$$S(q, \alpha, t) = W(q, \alpha) - \alpha t.$$

The equation

$$H + \frac{\partial S}{\partial t} = 0,$$

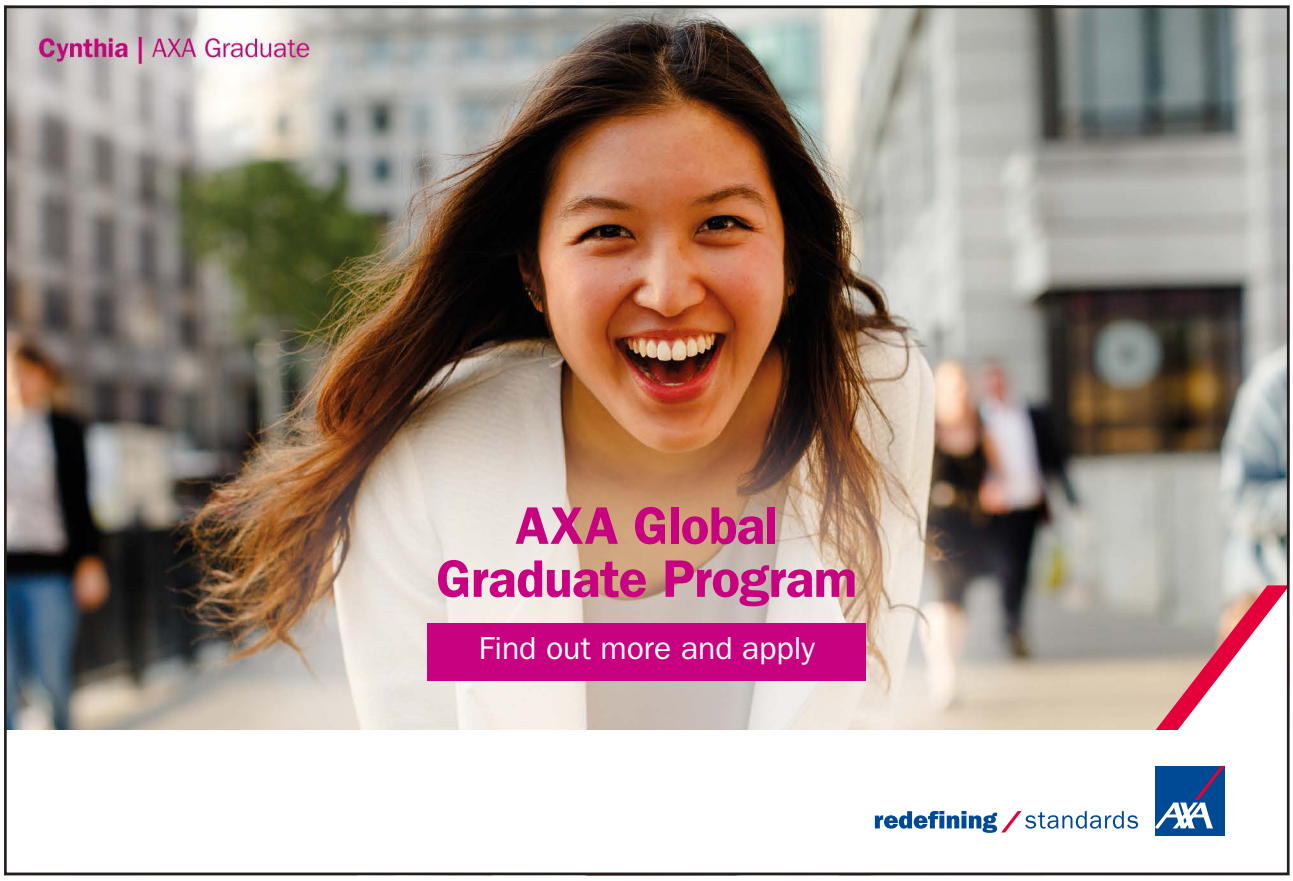
$$H + \underbrace{\frac{\partial W}{\partial t}}_{=0} - \alpha = 0,$$

means that

$$H = E = \alpha = \text{total energy}.$$

Thus, for a conservative system,

$$S(q, \alpha, t) = W(q, \alpha) - Et. \tag{8.27}$$



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Conclusion: for a conservative system the Hamilton-Jacobi equation (8.23) yields that

$$H(q,\alpha) = E, \tag{8.28}$$

with

$$\alpha_i = \frac{\partial S}{\partial q_i} = \frac{\partial W}{\partial q_i}. \tag{8.29}$$

Here W is called **Hamilton's characteristic function**.

Example 24. Harmonic oscillator. Consider the Hamilton function for the harmonic oscillator:

$$H = \frac{p^2}{2m} + \frac{1}{2}kq^2.$$

With $p = \frac{\partial S}{\partial q}$ the condition $H + \frac{\partial S}{\partial t} = 0$ gives that

$$\frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + \frac{1}{2}kq^2 + \frac{\partial S}{\partial t} = 0.$$

Since H does not depend on time we have $S(q,\alpha,t) = W(q,\alpha) - \alpha t$, implying

$$\frac{1}{2m}\left(\frac{\partial W}{\partial q}\right)^2 + \frac{kq^2}{2} = \alpha$$

$$W = \sqrt{mk}\int dq\sqrt{\frac{2\alpha}{k} - q^2}$$

$$S = \sqrt{mk}\int dq\sqrt{\frac{2\alpha}{k} - q^2} - \alpha t,$$

which is Hamilton's principal function. Of physical importance are only the partial derivatives of S. As in the text above we define

$$Q \equiv \beta' = \frac{\partial S}{\partial \alpha} = \sqrt{\frac{m}{k}}\int \frac{dq}{\sqrt{\frac{2\alpha}{k} - q^2}} - t$$

$$t + \beta' = +\sqrt{\frac{m}{k}}\arcsin\left(k\sqrt{\frac{k}{2\alpha}}\right)$$

$$q = \frac{2\alpha}{k}\sin(\omega t + \beta),$$

where $\beta = \beta'\omega$, $\omega \equiv \sqrt{\frac{m}{k}}$, and $\alpha = E$.

Consider finally the momentum:

$$p = \frac{\partial S}{\partial q} = \sqrt{mk}\sqrt{\frac{2\alpha}{k} - q^2} = \sqrt{mk}\sqrt{\frac{2\alpha}{k} - \frac{2\alpha}{k}\sin^2(\omega t + \beta)}$$

$$p = \sqrt{2m\alpha}\cos(\omega t + \beta).$$

We see that this agrees with the relation $p = m\dot{q}$.

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